

# **The Transport and Deposition of Persistent Toxic Substances to the Great Lakes**

## **I. The Capability of Specific Persistent Toxic Substances to be Subjected to Long Range Atmospheric Transport**

**Final Draft  
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**prepared for the International Joint Commission's  
International Air Quality Advisory Board**

**by**

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## **Appendix A.**

### **Physical-Chemical Properties**

NAME		Molecular Formula and Weight				PHYSICAL STATE	
common chemical name	IUPAC #	cas # (1)	molecular formula	calc'd weight	rept'd weight	(probably at room temperature)	"physical state" reference
octachlorostyrene	029082-74-4		C8 Cl8	379.7	379.68		
4-bromophenyl phenyl ether	000101-55-3		C6H5-O-C6H4Br	249.1	249.11	varies; Tm ~ 18 deg C	considering Tm
3,3'-dichlorobenzidine	000091-94-1		C12 H10 Cl2 N2	253.1	253.13	solid	considering Tm; also stated by ATSDR citing HSDB
1,3-dinitropyrene	075321-20-9		C16 H8 N2 O4	292.3	292.25	probably solid	considering Tm of 1,6 DNP
1,6-dinitropyrene	042397-64-8		C16 H8 N2 O4	292.3	292.25	probably solid	considering Tm of 1,6 DNP
1,8-dinitropyrene	042397-65-9		C16 H8 N2 O4	292.3	292.25	probably solid	considering Tm of 1,6 DNP
2,7-dinitropyrene	117929-15-4		C16 H8 N2 O4	292.3	292.25	probably solid	considering Tm of 1,6 DNP
dinitropyrenes (mixed)	078432-19-6		C16 H8 N2 O4	292.3	292.25	probably solid	considering Tm of 1,6 DNP
hexachloro-1,3-butadiene	000087-68-3		C4 Cl6	260.7	260.76	liquid	99; consistent with Tm
4,4'-methylene bis(2-chloroaniline)	000101-14-4		C13 H12 Cl2 N2	267.2	267	solid	considering Tm
pentachlorophenol	000087-86-5		C6 H Cl5 O	266.3	266.34	flakes or crystalline solid	42; also consistent with Tm
aldrin	000309-00-2		C12 H8 Cl6	364.9	364.93	crystalline solid	47; also consistent with Tm
diechlorin	000060-57-1		C12 H8 Cl6 O	380.9	380.93	crystalline solid	47; also consistent with Tm
p,p'-DDT	000050-29-3		(C1C6H4)2CHClCl3	354.5	354.49	crystalline solid	59; also consistent with Tm
p,p'-DDD	000072-54-8		(C1C6H4)2CHCHCl2	320.0	320.05	crystalline solid	60; also consistent with Tm
p,p'-DDE	000072-55-9		(C1C6H4)2C=CCl2	318.0	318.03	crystalline solid	60; also consistent with Tm
heptachlor	000076-44-8		C10 H5 Cl7	373.3	373.35	crystalline solid	53; also consistent with Tm
heptachlor epoxide	001024-57-3		C10 H5 Cl7 O	389.3	389.4	crystalline solid	53; note: ref 52 says that its liquid...; but if melted
methoxychlor	000072-43-5		C16 H15 Cl3 O2	345.6	345.65	solid	considering Tm
mirex	002385-85-5		C10 Cl12	545.5	545.59	crystalline solid	65; also consistent with Tm
toxaphene	008001-35-2		approx C10 H10 Cl8	413.8	414 (avg)	waxy solid	42; also consistent with Tm
endrin	000072-20-8		C12 H8 Cl6 O	380.9	380.92	crystalline solid	42; also consistent with Tm
alpha-hexachlorocyclohexane	000319-84-6		C6 H6 Cl6	290.8	290.83	crystalline solid	32; also consistent with Tm
beta-hexachlorocyclohexane	000319-85-7		C6 H6 Cl6	290.8	290.83	crystalline solid	33; also consistent with Tm
delta-hexachlorocyclohexane	000319-86-8		C6 H6 Cl6	290.8	290.83	fine plates	29; also consistent with Tm
gamma-hexachlorocyclohexane	000058-89-9		C6 H6 Cl6	290.8	290.83	crystalline solid	33; also consistent with Tm
mixed hexachlorocyclohexanes	000319-84-6		C6 H6 Cl6	290.8	290.83		

common chemical name	IUPAC #	cas # (1)	formula	Molecular Formula and Weight		calc'd molecular	rept'd molecular	molecular	at room temperature)	reference	PHYSICAL STATE
				weight	weight						
cadmium	007440-43-9	Cd	112.4	112.4		solid	71; also consistent with Tm				
cadmium carbonate	000513-78-0	CdCO <sub>3</sub>	172.4	172.42		solid	71; also consistent with Tm				
cadmium chloride	010108-64-2	CdCl <sub>2</sub>	183.3	183.32		solid	71; also consistent with Tm				
cadmium oxide	001306-19-0	CdO	128.4	128.41		solid	71; also consistent with Tm				
cadmium sulfate	010124-36-4	CdSO <sub>4</sub>	208.5	208.47		solid	71; also consistent with Tm				
cadmium sulfide	001306-23-6	CdS	144.5	144.47		solid	71; also consistent with Tm				
elemental mercury	007439-97-6	Hg	200.59	200.59		liquid				94	
mercury oxide	021908-53-2	HgO									
mercuric chloride	007487-94-7	Hg Cl <sub>2</sub>	271.49			solid				94	
monomethyl mercury chloride	000115-09-3	CH <sub>3</sub> Hg Cl	251.08	251.08		solid	95; also consistent with Tm				
dimethyl mercury	000593-74-8	CH <sub>3</sub> Hg CH <sub>3</sub>									
tetraethyl lead	000078-00-2	C <sub>8</sub> H <sub>20</sub> Pb	323.4	323.44		probably liquid	melting point is -136 deg C; boiling point is ~ 215 C				
tetramethyl lead	000075-74-1	C <sub>4</sub> H <sub>12</sub> Pb	267.3			liquid	hsdb				
triethyl lead radical (1+ cation)	014570-15-1	C <sub>6</sub> H <sub>15</sub> Pb (1+)	294.4								
triethyl lead hydride	005224-23-7	C <sub>6</sub> H <sub>16</sub> Pb	295.4								
triethyl lead chloride	001067-14-7	C <sub>6</sub> H <sub>15</sub> Cl Pb	329.8								
diethyl lead radical (2+ cation)	024952-65-6	C <sub>4</sub> H <sub>10</sub> Pb (2+)	265.3								
diethyl lead dihydride	081494-11-3	C <sub>4</sub> H <sub>12</sub> Pb	267.3								
diethyl lead dichloride	013231-90-8	C <sub>4</sub> H <sub>10</sub> Cl <sub>2</sub> Pb	336.2								
trimethyl lead radical (1+ cation)	014570-16-2	C <sub>3</sub> H <sub>9</sub> Pb (1+)	252.3								
trimethyl lead hydride	007442-13-9	C <sub>3</sub> H <sub>10</sub> Pb	253.3								
trimethyl lead chloride	001520-78-1	C <sub>3</sub> H <sub>9</sub> Cl Pb	287.8								
dimethyl lead radical (2+ cation)	021774-13-0	C <sub>2</sub> H <sub>6</sub> Pb (2+)	237.3								
dimethyl lead dihydride	030691-92-0	C <sub>2</sub> H <sub>8</sub> Pb	239.3								
dimethyl lead dichloride	001520-77-0	C <sub>2</sub> H <sub>6</sub> Cl <sub>2</sub> Pb	308.2								
bis (tributyltin) oxide	000056-35-9	C <sub>24</sub> H <sub>54</sub> O Sn <sub>2</sub>	595.62			liquid			97		
tributyl tin	000688-75-3										
tributyltin fluoride	001983-10-4	C <sub>12</sub> H <sub>27</sub> F Sn									
tributyltin chloride	001461-22-9	C <sub>12</sub> H <sub>27</sub> Cl Sn									
tributyltin hydroxide	001067-97-6	C <sub>12</sub> H <sub>28</sub> O Sn									
tributyltin naphthenate											
tris(tributylstanny) phosphate	013435-05-7										

NAME	Molecular Formula and Weight					PHYSICAL STATE
	IUPAC #	cas # (1)	formula	calc'd weight	rept'd weight	
			molecular	molecular	molecular	"physical state"
						(probably
						at room
common chemical name			formula	weight	weight	temperature)
						reference
1,4-dichlorobenzene	000106-46-7		C6 H4 Cl2	147.0	147.01	solid considering Tm
1,2,3,4-tetrachlorobenzene	000634-66-2		C6 H2 Cl4	215.9	215.89	solid considering Tm
1,2,4,5-tetrachlorobenzene	000095-94-3		C6 H2 Cl4	215.9	215.89	solid considering Tm
1,2,3,5-tetrachlorobenzene	000634-90-2		C6 H2 Cl4	215.9	215.89	solid considering Tm
pentachlorobenzene	000608-93-5		C6 H Cl5	250.3	250.34	solid considering Tm
hexachlorobenzene	000118-74-1		C6 Cl6	284.8	284.78	solid considering Tm
naphthalene	000091-20-3		C8 H10	106.2	128.19	solid considering Tm
acenaphthene	000083-32-9		C12 H10	154.2	154.21	solid considering Tm
acenaphthylene	000208-96-8		C12 H8	152.2	150.2	solid considering Tm
fluorene	000086-73-7		C13 H10	166.2	166.2	solid considering Tm
phenanthrene	000085-01-8		C14 H10	178.2	178.2	solid considering Tm
anthracene	000120-12-7		C14 H10	178.2	178.2	solid considering Tm
pyrene	000129-00-0		C16 H10	202.3	202.3	solid considering Tm
floranthene	000206-44-0		C16 H10	202.3	202.3	solid considering Tm
chrysene	000218-01-9		C18 H12	228.3	228.3	solid considering Tm
benz [ a ] anthracene	000056-55-3		C18 H12	228.3	228.3	solid ??? considering Tm from ref 6; but ref 85 gives Tm of -1
benzo [ b ] fluoranthene	000205-99-2		C20 H12	252.3	252.3	solid considering Tm
benzo [ j ] fluoranthene	000205-82-3		C20 H12	252.3	252.3	solid considering Tm
benzo [ k ] fluoranthene	000207-08-9		C20 H12	252.3	252.3	solid considering Tm
benzo [ a ] pyrene	000050-32-8		C20 H12	252.3	252.3	solid considering Tm
benzo [ e ] pyrene	000192-97-2		C20 H12	252.3	252.3	solid considering Tm
perylene	000198-55-0		C20 H12	252.3	252.3	solid considering Tm
benzo [ g,h,i ] perylene	000191-24-2		C21 H16	268.4	268.36	solid considering Tm
dibenz [ a,h ] anthracene	000053-70-3		C22 H14	278.4	278.35	solid considering Tm
indeno [ 1,2,3-c,d ] pyrene	000193-39-5		C22 H12	276.3	276.3	solid considering Tm

NAME	Molecular Formula and Weight					PHYSICAL STATE
						"physical state"
		calc'd	rept'd			(probably)
		molecular	molecular	molecular		at room
common chemical name	IUPAC #	cas # (1)	formula	weight	weight	temperature)
						reference
2,3,7,8-TCDD	001746-01-6	C12 H4 O2 Cl4	322.0	322	solid	considering Tm
1,2,3,7,8-PeCDD	040321-76-4	C12 H3 O2 Cl5	356.4	356.4	solid	considering Tm
1,2,3,4,7,8-HxCDD	039227-28-6	C12 H2 O2 Cl6	390.8	391	solid	considering Tm
1,2,3,6,7,8-HxCDD	057653-85-7	C12 H2 O2 Cl6	390.8	391	solid	considering Tm
1,2,3,7,8,9-HxCDD	019408-74-3	C12 H2 O2 Cl6	390.8	391	solid	considering Tm
1,2,3,4,6,7,8-HpCDD	035822-46-9	C12 H1 O2 Cl7	425.3	425.2	solid	considering Tm
OCDD	003268-87-9	C12 H0 O2 Cl8	459.7	460	solid	considering Tm
2,3,7,8-TCDF	051207-31-9	C12 H4 O Cl4	306.0	306	solid	considering Tm
2,3,4,7,8-PeCDF	057117-31-4	C12 H3 O Cl5	340.4	340.42	solid	considering Tm
1,2,3,7,8-PeCDF	057117-41-6	C12 H3 O Cl5	340.4	340.42	solid	considering Tm
1,2,3,4,7,8-HxCDF	070648-26-9	C12 H2 O Cl6	374.8	374.87	solid	considering Tm
1,2,3,6,7,8-HxCDF	057117-44-9	C12 H2 O Cl6	374.8	374.87	solid	considering Tm
1,2,3,7,8,9-HxCDF	072918-21-9	C12 H2 O Cl6	374.8	374.87	solid	considering Tm
2,3,4,6,7,8-HxCDF	060851-34-5	C12 H2 O Cl6	374.8	374.87	solid	considering Tm
1,2,3,4,6,7,8-HpCDF	067562-39-4	C12 H1 O Cl7	409.3	409.31	solid	considering Tm
1,2,3,4,7,8,9-HpCDF	055673-89-7	C12 H1 O Cl7	409.3	409.31	solid	considering Tm
OCDF	039001-02-0	C12 H0 O Cl8	443.7	443.8	solid	considering Tm

Molecular Formula and Weight							PHYSICAL STATE
common chemical name	IUPAC #	cas # (1)	molecular formula	calc'd weight	rept'd weight	"physical state"	(probably at room temperature) reference
biphenyl	0	000092-52-4	C12 H10	154.2	154.2	solid	considering Tm
2-PCB	1	002051-60-7	C12 H9 Cl	188.7	188.7	varies	Tm near room temp
3-PCB	2	002051-61-8	C12 H9 Cl	188.7	188.7	varies	Tm near room temp
4-PCB	3	002051-62-9	C12 H9 Cl	188.7	188.7	solid	considering Tm
count							
average							
standard deviation							
minimum							
maximum							
2,2'-PCB	4	013029-08-8	C12 H8 Cl2	223.1	223.1	solid	considering Tm
2,3-PCB	5	016605-91-7	C12 H8 Cl2	223.1	223.1	oil	96
2,4-PCB	7	033284-50-3	C12 H8 Cl2	223.1	223.1	varies	Tm near room temp
2,4'-PCB	8	034883-43-7	C12 H8 Cl2	223.1	223.1	solid	considering Tm
2,5-PCB	9	034883-39-1	C12 H8 Cl2	223.1	223.1	varies	Tm near room temp
2,6-PCB	10	033146-45-1	C12 H8 Cl2	223.1	223.1	varies	Tm near room temp
3,3'-PCB	11	002050-67-1	C12 H8 Cl2	223.1	223.1	varies	Tm near room temp
3,4-PCB	12	002974-92-7	C12 H8 Cl2	223.1	223.1	solid	considering Tm
3,5-PCB	14	034883-41-5	C12 H8 Cl2	223.1	223.1	varies	Tm near room temp
4,4'-PCB	15	002050-68-2	C12 H8 Cl2	223.1	223.1	solid	considering Tm
count							
average							
standard deviation							
minimum							
maximum							

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common chemical name	IUPAC #	cas # (1)	molecular formula	calc'd weight	rept'd weight	"physical state"	
						(probably at room temperature)	reference
2,2',3-PCB	16	038444-78-9	C12 H7 Cl3	257.5	257.5	varies	Tm near room temp
2,2',5-PCB	18	037680-65-2	C12 H7 Cl3	257.5	257.5	solid	considering Tm
2,3,3'-PCB	20	038444-84-7	C12 H7 Cl3	257.5	257.5	solid	solid, considering Tm
2,3,4-PCB	21	055702-46-0	C12 H7 Cl3	257.5	257.5	solid	considering Tm
2,3',5-PCB	26	038444-85-8	C12 H7 Cl3	257.5	257.5	solid	considering Tm
2,4,4'-PCB	28	007012-37-5	C12 H7 Cl3	257.5	257.5	solid	considering Tm
2,4,5-PCB	29	015862-07-4	C12 H7 Cl3	257.5	257.5	solid	considering Tm
2,4,6-PCB	30	035693-92-6	C12 H7 Cl3	257.5	257.5	solid	considering Tm
2,4',5,-PCB	31	016606-02-3	C12 H7 Cl3	257.5	257.5	solid	considering Tm
2',3,4-PCB	33	038444-86-9	C12 H7 Cl3	257.5	257.5	solid	considering Tm
3,3',4-PCB	35	037680-69-6	C12 H7 Cl3	257.5	257.5	solid	considering Tm
3,4,4'-PCB	37	038444-90-5	C12 H7 Cl3	257.5	257.5	solid	considering Tm
count							
average							
standard deviation							
minimum							
maximum							
2,2',3,3'-PCB	40	038444-93-8	C12 H6 Cl4	292.0	292.0	solid	considering Tm
2,2',3,5'-PCB	44	041464-39-5	C12 H6 Cl4	292.0	292.0	solid	considering Tm
2,2',4,4'-PCB	47	002437-79-8	C12 H6 Cl4	292.0	292.0	solid	considering Tm
2,2',4,5'-PCB	49	041464-40-8	C12 H6 Cl4	292.0	292.0	solid	considering Tm
2,2',4,6-PCB	50	062796-65-0	C12 H6 Cl4	292.0	292.0	solid	considering Tm
2,2',4,6'-PCB	51	068194-04-7	C12 H6 Cl4	292.0	292.0	oil	95
2,2,5,5'-PCB	52	035693-99-3	C12 H6 Cl4	292.0	292.0	solid	considering Tm
2,2,5,6'-PCB	53	041464-41-9	C12 H6 Cl4	292.0	292.0	solid	considering Tm
2,2,6,6'-PCB	54	015968-05-5	C12 H6 Cl4	292.0	292.0	solid	considering Tm
2,3,4,4'-PCB	60	033025-41-1	C12 H6 Cl4	292.0	292.0	solid	considering Tm
2,3,4,5-PCB	61	033284-53-6	C12 H6 Cl4	292.0	292.0	solid	considering Tm
2,3,5,6-PCB	65	033284-54-7	C12 H6 Cl4	292.0	292.0	solid	considering Tm
2,3,4,4'-PCB	66	032598-10-0	C12 H6 Cl4	292.0	292.0	solid	considering Tm
2,3',4',5-PCB	70	032598-11-1	C12 H6 Cl4	292.0	292.0	solid	considering Tm
2,4,4',6-PCB	75	032598-12-2	C12 H6 Cl4	292.0	292.0	solid	considering Tm
3,3',4,4'-PCB	77	032598-13-3	C12 H6 Cl4	292.0	292.0	solid	considering Tm
3,3',5,5'-PCB	80	033284-52-5	C12 H6 Cl4	292.0	292.0	solid	considering Tm
3,4,4',5-PCB	81	070362-50-4	C12 H6 Cl4	292.0	292.0	solid	considering Tm
count							
average							
standard deviation							
minimum							
maximum							

common chemical name	IUPAC #	cas # (1)	Molecular Formula and Weight			calc'd molecular formula	rept'd molecular weight	at room temperature)	reference	PHYSICAL STATE
			"physical state"	(probably at room temperature)						
2,2',3,3',5-PCB	83	060145-20-2	C12 H5 Cl5	326.4	326.4	solid	considering Tm			
2,2',3,4,5-PCB	86	065510-45-4	C12 H5 Cl5	326.4	326.4	solid	considering Tm			
2,2',3,4,5'-PCB	87	038380-02-8	C12 H5 Cl5	326.4	326.4	solid	considering Tm			
2,2',3,4,6-PCB	88	055215-17-3	C12 H5 Cl5	326.4	326.4	solid	considering Tm			
2,2',3,5,6-PCB	95	038379-99-6	C12 H5 Cl5	326.4	326.4	solid	considering Tm			
2,2',4,4,5-PCB	99	038380-01-7	C12 H5 Cl5	326.4	326.4	solid	considering Tm			
2,2',4,4,6-PCB	100	039485-83-1	C12 H5 Cl5	326.4	326.4	oil		95		
2,2',4,5,5'-PCB	101	037680-73-2	C12 H5 Cl5	326.4	326.4	solid	considering Tm			
2,2',4,6,6'-PCB	104	056558-16-8	C12 H5 Cl5	326.4	326.4	solid	considering Tm			
2,3,3',4,4'-PCB	105	032598-14-1	C12 H5 Cl5	326.4	326.4	solid	considering Tm			
2,3,3',4,6-PCB	110	038380-03-9	C12 H5 Cl5	326.4	326.4	solid	considering Tm			
2,3,4,4',5-PCB	114	074472-37-0	C12 H5 Cl5	326.4	326.4	solid	considering Tm			
2,3,4,5,6-PCB	116	018259-05-7	C12 H5 Cl5	326.4	326.4	solid	considering Tm			
2,3',4,4',5-PCB	118	031508-00-6	C12 H5 Cl5	326.4	326.4	solid	considering Tm			
2,3,4,5,5'-PCB	124	070424-70-3	C12 H5 Cl5	326.4	326.4	solid	considering Tm			
3,3',4,4',5-PCB	126	057465-28-8	C12 H5 Cl5	326.4	326.4	solid	considering Tm			
count										
average										
standard deviation										
minimum										
maximum										
2,2',3,3',4,4'-PCB	128	038380-07-3	C12 H4 Cl6	360.9	360.9	solid	considering Tm			
2,2',3,3',4,5-PCB	129	055215-18-4	C12 H4 Cl6	360.9	360.9	solid	considering Tm			
2,2',3,3',5,6-PCB	134	052704-70-8	C12 H4 Cl6	360.9	360.9	solid	considering Tm			
2,2',3,3',6,6'-PCB	136	038411-22-2	C12 H4 Cl6	360.9	360.9	solid	considering Tm			
2,2',3,4,4',5-PCB	138	035065-28-2	C12 H4 Cl6	360.9	360.9	solid	considering Tm			
2,2',3,4',5,6-PCB	149	038380-04-0	C12 H4 Cl6	360.9	360.9	solid	considering Tm			
2,2',4,4',5,5'-PCB	153	035065-27-1	C12 H4 Cl6	360.9	360.9	solid	considering Tm			
2,2',4,4',6,6'-PCB	155	033979-03-2	C12 H4 Cl6	360.9	360.9	solid	considering Tm			
2,3,3',4,4',5-PCB	156	038380-08-4	C12 H4 Cl6	360.9	360.9	solid	considering Tm			
2,3,3',4,4',5'-PCB	157	069782-90-7	C12 H4 Cl6	360.9	360.9	solid	considering Tm			
2,3',4,4',5,5'-PCB	167	052663-72-6	C12 H4 Cl6	360.9	360.9	solid	considering Tm			
3,3',4,4',5,5'-PCB	169	032774-16-6	C12 H4 Cl6	360.9	360.9	solid	considering Tm			
count										
average										
standard deviation										
minimum										
maximum										

NAME		Molecular Formula and Weight				PHYSICAL STATE	
common chemical name	IUPAC #	cas # (1)	formula	calc'd molecular	rept'd molecular	at room temperature)	"physical state" (probably) reference
2,2',3,3',4,4',5-PCB	170	035065-30-6	C12 H3 Cl7	395.3	395.3	solid	considering Tm
2,2',3,3',4,4',6-PCB	171	052663-71-5	C12 H3 Cl7	395.3	395.3	solid	considering Tm
2,2',3,4,4',5,5'-PCB	180	035065-29-3	C12 H3 Cl7	395.3	395.3	solid	considering Tm
2,2',3,4,5,5',6-PCB	185	052712-05-7	C12 H3 Cl7	395.3	395.3	solid	considering Tm
2,2',3,4,5,5',6-PCB	187	052663-68-0	C12 H3 Cl7	395.3	395.3	solid	considering Tm
2,3,3',4,4',5,5'-PCB	189	039635-31-9	C12 H3 Cl7	395.3	395.3	solid	considering Tm
count							
average							
standard deviation							
minimum							
maximum							
2,2',3,3',4,4',5,5'-PCB	194	035694-08-7	C12 H2 Cl8	429.7	429.7	solid	considering Tm
2,2',3,3',5,5',6,6'-PCB	202	002136-99-4	C12 H2 Cl8	429.7	429.7	solid	considering Tm
count							
average							
standard deviation							
minimum							
maximum							
2,2',3,3',4,4',5,5',6-PCB	206	040186-72-9	C12 H Cl9	464.2	464.2	solid	considering Tm
2,2',3,3',4,4',5,6,6'-PCB	207	052663-79-3	C12 H Cl9	464.2	464.2	solid	considering Tm
2,2',3,3',4,5,5',6,6'-PCB	208	052663-77-1	C12 H Cl9	464.2	464.2	solid	considering Tm
count							
average							
standard deviation							
minimum							
maximum							
2,2',3,3',4,4',5,5',6,6'-PCB	209	002051-24-3	C12 Cl10	498.6	498.6	solid	considering Tm

NAME	IUPAC #	cas # (1)	range	average	units	ref	MELTING POINT	
							melting point	for V/P
common chemical name							melting	
octachlorostyrene	029082-74-4			150	deg C	89	423	estimated using linear regression; not in SRC database
4-bromophenyl phenyl ether	000101-55-3			18	deg C	7	291.15	
3,3'-dichlorobenzidine	000091-94-1		132-133	132.5	deg C	Howard, Volume 1	405.65	same in ref 8; & ATSDR
1,3-dinitropyrene	075321-20-9						479.15	crude: pyrene+50 C
1,6-dinitropyrene	042397-64-8		> 300		deg C	aldrich catalog, pag	479.15	crude: pyrene+50 C
1,8-dinitropyrene	042397-65-9						479.15	crude: pyrene+50 C
2,7-dinitropyrene	117929-15-4						479.15	crude: pyrene+50 C
dinitropyrenes (mixed)	078432-19-6						479.15	crude: pyrene+50 C
hexachloro-1,3-butadiene	000087-68-3			-21	deg C	7; 99	252.15	
4,4'-methylene bis(2-chloroaniline)	000101-14-4			110	deg C	15	383.15	
pentachlorophenol	000087-86-5			174	deg C	8	447.15	
aldrin	000309-00-2			104	deg C	25	377.15	
dielein	000060-57-1		175-176	175.5	deg C	25	448.65	
p,p'-DDT	000050-29-3		107-110	108.5	deg C?	aldrich catalog, pag	381.65	same in ref 61
p,p'-DDD	000072-54-8		109-111	110	deg C?	aldrich catalog, pag	383.15	same in ref 61
p,p'-DDE	000072-55-9		88-90	89	deg C?	aldrich catalog, pag	362.15	same in ref 61 and SRC data set
heptachlor	000076-44-8		95-96	95.5	deg C	25	368.65	same in ref 85
heptachlor epoxide	001024-57-3		160-161.5	160.75	deg C	25	433.9	same in ref 85
methoxychlor	000072-43-5			89	deg C	24; 85	362.15	
mirex	002385-85-5			485	deg C	65	758.15	decomposes
toxaphene	008001-35-2		65 - 90	77.5	deg C	25	350.65	
endrin	000072-20-8		226-230	228	deg C	25	501.15	decomposes when melted
alpha-hexachlorocyclohexane	000319-84-6			159.5	deg C	29	432.65	
beta-hexachlorocyclohexane	000319-85-7			314.5	deg C	29	587.65	
delta-hexachlorocyclohexane	000319-86-8			141.5	deg C	29	414.65	
gamma-hexachlorocyclohexane	000058-89-9			112.5	deg C	29, 30	385.65	
mixed hexachlorocyclohexanes	000319-84-6							

common chemical name	IUPAC #	cas # (1)	range	average	units	ref	MELTING POINT		notes
							melting	melting	
							point	point	
cadmium	007440-43-9			320.9	deg C		594.05		71
cadmium carbonate	000513-78-0		decomposes at less than 500	deg C					72
cadmium chloride	010108-64-2			568	deg C		841.15		71
cadmium oxide	001306-19-0		less than 1426	deg C					73
cadmium sulfate	010124-36-4			1000	deg C		1273.15		71
cadmium sulfide	001306-23-6			1475	deg C		1748.15		74
elemental mercury	007439-97-6			-38.87	deg C	94	234.28		
mercury oxide	021908-53-2								
mercuric chloride	007487-94-7			276	deg C	94	549.15		
monomethyl mercury chloride	000115-09-3			170	deg C	95	443.15		
dimethyl mercury	000593-74-8								
tetraethyl lead	000078-00-2			-136	deg C	85	137.15		
tetramethyl lead	000075-74-1			-27.5	deg C	97	245.65		
triethyl lead radical (1+ cation)	014570-15-1								
triethyl lead hydride	005224-23-7								
triethyl lead chloride	001067-14-7								
diethyl lead radical (2+ cation)	024952-65-6								
diethyl lead dihydride	081494-11-3								
diethyl lead dichloride	013231-90-8								
trimethyl lead radical (1+ cation)	014570-16-2								
trimethyl lead hydride	007442-13-9								
trimethyl lead chloride	001520-78-1								
dimethyl lead radical (2+ cation)	021774-13-0								
dimethyl lead dihydride	030691-92-0								
dimethyl lead dichloride	001520-77-0								
bis (tributyltin) oxide	000056-35-9			-45	deg C	97	228.15	ref says "solidifies below -45 C"	
tributyl tin	000688-75-3								
tributyltin fluoride	001983-10-4								
tributyltin chloride	001461-22-9								
tributyltin hydroxide	001067-97-6								
tributyltin naphthenate									
tris(tributylstanny) phosphate	013435-05-7								

common chemical name	IUPAC #	cas # (1)	range	average	units	ref	MELTING POINT		notes
							melting	melting	
							point	point	
1,4-dichlorobenzene	000106-46-7			53.1	deg C	5	326.25	similar in Aldrich catalog	
1,2,3,4-tetrachlorobenzene	000634-66-2			47.5	deg C	5	320.65	similar in Aldrich catalog	
1,2,4,5-tetrachlorobenzene	000095-94-3			140	deg C	5	413.15	similar in Aldrich catalog	
1,2,3,5-tetrachlorobenzene	000634-90-2			54.5	deg C	5	327.65		
pentachlorobenzene	000608-93-5			86	deg C	5	359.15	similar in Aldrich catalog	
hexachlorobenzene	000118-74-1			230	deg C	5	503.15	similar in Aldrich catalog	
naphthalene	000091-20-3			80.5	deg C	6	353.65		
acenaphthene	000083-32-9			96.2	deg C	6	369.35		
acenaphthylene	000208-96-8			92	deg C	6	365.15		
fluorene	000086-73-7			116	deg C	6	389.15		
phenanthrene	000085-01-8			101	deg C	6	374.15		
anthracene	000120-12-7			216.2	deg C	6	489.35		
pyrene	000129-00-0			156	deg C	6	429.15		
floranthene	000206-44-0			111	deg C	6	384.15		
chrysene	000218-01-9			255	deg C	6	528.15		
benz [ a ] anthracene	000056-55-3			160	deg C	6	433.15		
benzo [ b ] fluoranthene	000205-99-2			168	deg C	6	441.15		
benzo [ j ] fluoranthene	000205-82-3			166	deg C	6	439.15		
benzo [ k ] fluoranthene	000207-08-9			217	deg C	6	490.15		
benzo [ a ] pyrene	000050-32-8			175	deg C	6	448.15		
benzo [ e ] pyrene	000192-97-2			178	deg C	6	451.15		
perylene	000198-55-0			277	deg C	6	550.15		
benzo [ g,h,i ] perylene	000191-24-2			277	deg C	6	550.15		
dibenz [ a,h ] anthracene	000053-70-3			267	deg C	6	540.15		
indeno [ 1,2,3-c,d ] pyrene	000193-39-5			163.6	deg C	9	436.75		

common chemical name	IUPAC #	cas # (1)	range	average	units	ref	MELTING POINT	
							melting point	for V/P
2,3,7,8-TCDD	001746-01-6			305	deg C	6	578.15	
1,2,3,7,8-PeCDD	040321-76-4			195	deg C	6	468.15	using value for 12347 PeCDD
1,2,3,4,7,8-HxCDD	039227-28-6			273	deg C	6	546.15	
1,2,3,6,7,8-HxCDD	057653-85-7			273	deg C	6	546.15	using value for 123478 HxCDD
1,2,3,7,8,9-HxCDD	019408-74-3			273	deg C	6	546.15	using value for 123478 HxCDD
1,2,3,4,6,7,8-HpCDD	035822-46-9			265	deg C	6	538.15	
OCDD	003268-87-9			322	deg C	6	595.15	
2,3,7,8-TCDF	051207-31-9			227	deg C	6	500.15	
2,3,4,7,8-PeCDF	057117-31-4			196	deg C	6	469.15	
1,2,3,7,8-PeCDF	057117-41-6			196	deg C	6	469.15	using value for 23478 PeCDF
1,2,3,4,7,8-HxCDF	070648-26-9			225.5	deg C	6	498.65	
1,2,3,6,7,8-HxCDF	057117-44-9			232	deg C	6	505.15	
1,2,3,7,8,9-HxCDF	072918-21-9			228.75	deg C	6	501.9	using avg of values for 123478 HxCDF and 123678 HxCDF
2,3,4,6,7,8-HxCDF	060851-34-5			228.75	deg C	6	501.9	using avg of values for 123478 HxCDF and 123678 HxCDF
1,2,3,4,6,7,8-HpCDF	067562-39-4			236	deg C	6	509.15	
1,2,3,4,7,8,9-HpCDF	055673-89-7			221	deg C	6	494.15	
OCDF	039001-02-0			258	deg C	6	531.15	

NAME							MELTING POINT	
							for V/P	
							melting	
common chemical name	IUPAC #	cas # (1)	range	average	units	ref	point	data
biphenyl	0	000092-52-4		71	deg C	5	344.15	
2-PCB	1	002051-60-7		34	deg C	5	307.15	
3-PCB	2	002051-61-8		25.1	deg C	5	298.25	
4-PCB	3	002051-62-9		77.9	deg C	5	351.05	
count								
average								
standard deviation								
minimum								
maximum								
2,2'-PCB	4	013029-08-8		61	deg C	5	334.15	
2,3-PCB	5	016605-91-7		<i>not in ref 5, 85, or 95</i>		273.15	guess; since oil at room temp, must be less than room temp	
2,4-PCB	7	033284-50-3		24.4	deg C	5	297.55	
2,4'-PCB	8	034883-43-7		43	deg C	5	316.15	
2,5-PCB	9	034883-39-1		25.1	deg C	5	298.25	
2,6-PCB	10	033146-45-1		34.9	deg C	5	308.05	
3,3'-PCB	11	002050-67-1		29	deg C	5	302.15	
3,4-PCB	12	002974-92-7		49	deg C	5	322.15	
3,5-PCB	14	034883-41-5		31	deg C	5	304.15	
4,4'-PCB	15	002050-68-2		149	deg C	5	422.15	
count								
average								
standard deviation								
minimum								
maximum								

NAME							MELTING POINT									
							for V/P									
							melting	melting	melting	melting	melting	melting	point	point	point	data
common chemical name	IUPAC #	cas # (1)	range	average	units	ref	deg K	notes								
2,2',3-PCB	16	038444-78-9			28	deg C	5	301.15								
2,2',5-PCB	18	037680-65-2			44	deg C	5	317.15								
2,3,3'-PCB	20	038444-84-7		43 - 44.5	43.75	deg C	95	316.9								
2,3,4-PCB	21	055702-46-0			102	deg C	5	375.15								
2,3',5-PCB	26	038444-85-8			40.5	deg C	5	313.65								
2,4,4'-PCB	28	007012-37-5			57	deg C	5	330.15								
2,4,5-PCB	29	015862-07-4			78	deg C	5	351.15								
2,4,6-PCB	30	035693-92-6			62.5	deg C	5	335.65								
2,4',5,-PCB	31	016606-02-3			67	deg C	5	340.15								
2',3,4-PCB	33	038444-86-9			60	deg C	5	333.15								
3,3',4-PCB	35	037680-69-6			87	deg C	5	360.15								
3,4,4'-PCB	37	038444-90-5			87	deg C	5	360.15								
count																
average																
standard deviation																
minimum																
maximum																
2,2',3,3'-PCB	40	038444-93-8			121	deg C	5	394.15								
2,2',3,5'-PCB	44	041464-39-5			47	deg C	5	320.15								
2,2',4,4'-PCB	47	002437-79-8			83	deg C	5	356.15								
2,2',4,5'-PCB	49	041464-40-8			64	deg C	5	337.15								
2,2',4,6-PCB	50	062796-65-0		47 - 48	47.5	deg C	95	320.65								
2,2',4,6'-PCB	51	068194-04-7			<i>not in ref 5, 85, or 95</i>		273.15	guess; since oil at room temp, must be less than room temp								
2,2,5,5'-PCB	52	035693-99-3			87	deg C	5	360.15								
2,2,5,6'-PCB	53	041464-41-9			104	deg C	5	377.15								
2,2,6,6'-PCB	54	015968-05-5			198	deg C	5	471.15								
2,3,4,4'-PCB	60	033025-41-1			142	deg C	5	415.15								
2,3,4,5-PCB	61	033284-53-6			92	deg C	5	365.15								
2,3,5,6-PCB	65	033284-54-7			79	deg C	5	352.15								
2,3,4,4'-PCB	66	032598-10-0			124	deg C	5	397.15								
2,3',4',5-PCB	70	032598-11-1			104	deg C	5	377.15								
2,4,4',6-PCB	75	032598-12-2		62 - 63	62.5	deg C	95	335.65								
3,3',4,4'-PCB	77	032598-13-3			180	deg C	5	453.15								
3,3',5,5'-PCB	80	033284-52-5			164	deg C	5	437.15								
3,4,4',5-PCB	81	070362-50-4		160 - 163	161.5	deg C	95	434.65								
count																
average																
standard deviation																
minimum																
maximum																

NAME							MELTING POINT			
common chemical name	IUPAC #	cas # (1)	range	average	units	ref	melting point		data	
							melting point	melting point		
2,2',3,3',5-PCB	83	060145-20-2	83 - 84	83.5	deg C	95	356.65			
2,2',3,4,5-PCB	86	065510-45-4		100	deg C	5	373.15			
2,2',3,4,5'-PCB	87	038380-02-8		114	deg C	5	387.15			
2,2',3,4,6-PCB	88	055215-17-3		100	deg C	5	373.15			
2,2',3,5,6-PCB	95	038379-99-6		100	deg C	5	373.15			
2,2',4,4,5-PCB	99	038380-01-7	59 - 60	59.5	deg C	95	332.65			
2,2',4,4,6-PCB	100	039485-83-1		<i>not in ref 5, or 95</i>			273.15	<i>guess; since oil at room temp, must be less than room temp</i>		
2,2',4,5,5'-PCB	101	037680-73-2		76.5	deg C	5	349.65			
2,2',4,6,6'-PCB	104	056558-16-8	87 - 88	87.5	deg C	95	360.65			
2,3,3',4,4'-PCB	105	032598-14-4		105	deg C	5	378.15			
2,3,3',4,6-PCB	110	038380-03-9	53 - 55	54	deg C	95	327.15			
2,3,4,4',5-PCB	114	074472-37-0	111 - 113	112	deg C	95	385.15			
2,3,4,5,6-PCB	116	018259-05-7		124	deg C	5	397.15			
2,3',4,4',5-PCB	118	031508-00-6		107	deg C	5	380.15			
2',3,4,5,5'-PCB	124	070424-70-3	116 - 117	116.5	deg C	95	389.65			
3,3',4,4',5-PCB	126	057465-28-8	160 - 161	160.5	deg C	95	433.65			
count										
average										
standard deviation										
minimum										
maximum										
2,2',3,3',4,4'-PCB	128	038380-07-3		150	deg C	5	423.15			
2,2',3,3',4,5-PCB	129	055215-18-4		85	deg C	5	358.15			
2,2',3,3',5,6-PCB	134	052704-70-8		100	deg C	5	373.15			
2,2',3,3',6,6'-PCB	136	038411-22-2		112.2	deg C	5	385.35			
2,2',3,4,4',5'-PCB	138	035065-28-2		80	deg C	5	353.15			
2,2',3,4',5,6-PCB	149	038380-04-0	78-79	78.5	deg C	95	351.65	<i>reported as oil in ref 5</i>		
2,2',4,4',5,5'-PCB	153	035065-27-1		103	deg C	5	376.15			
2,2',4,4',6,6'-PCB	155	033979-03-2		114	deg C	5	387.15			
2,3,3',4,4',5-PCB	156	038380-08-4	129.5 - 131	130.25	deg C	95	403.4			
2,3,3',4,4',5'-PCB	157	069782-90-7	161 - 162	161.5	deg C	95	434.65			
2,3',4,4',5,5'-PCB	167	052663-72-6	125 - 127	126	deg C	95	399.15			
3,3',4,4',5,5'-PCB	169	032774-16-6		202	deg C	5	475.15			
count										
average										
standard deviation										
minimum										
maximum										

NAME							MELTING POINT		
							for V/P		
			melting	melting	melting	melting	melting	data	
common chemical name	IUPAC #	cas # (1)	range	average	units	ref	deg K	notes	
2,2',3,3',4,4',5-PCB	170	035065-30-6	136.5 - 138.5	137.5	deg C	95	410.65		
2,2',3,3',4,4',6-PCB	171	052663-71-5		122.4	deg C	5	395.55		
2,2',3,4,4',5,5'-PCB	180	035065-29-3		110	deg C	5	383.15		
2,2',3,4,5,5',6-PCB	185	052712-05-7		149	deg C	5	422.15		
2,2',3,4',5,5',6-PCB	187	052663-68-0	104 - 105	104.5	deg C	95	377.65		
2,3,3',4,4',5,5'-PCB	189	039635-31-9	162 - 163	162.5	deg C	95	435.65		
count									
average									
standard deviation									
minimum									
maximum									
2,2',3,3',4,4',5,5'-PCB	194	035694-08-7		159	deg C	5	432.15		
2,2',3,3',5,5',6,6'-PCB	202	002136-99-4		162	deg C	5	435.15		
count									
average									
standard deviation									
minimum									
maximum									
2,2',3,3',4,4',5,5',6-PCB	206	040186-72-9		206	deg C	5	479.15		
2,2',3,3',4,4',5,6,6'-PCB	207	052663-79-3	213 - 215	214	deg C	95	487.15		
2,2',3,3',4,5,5',6,6'-PCB	208	052663-77-1		182.8	deg C	5	455.95		
count									
average									
standard deviation									
minimum									
maximum									
2,2',3,3',4,4',5,5',6,6'-PCB	209	002051-24-3		305.9	deg C	5	579.05		

BOILING POINT									
NAME	IUPAC #	cas # (1)	range	average	units	ref	for V/P		
							boiling	point	data
common chemical name							deg K	notes	
octachlorostyrene		029082-74-4		379	deg C	89	652	estimated using linear regression; not in SRC database	
4-bromophenyl phenyl ether		000101-55-3		310	deg C	7	583.15		
3,3'-dichlorobenzidine		000091-94-1		420	deg C	18	693.15	368 deg C value given in ATSDR as an estimate, citing PCGEMS 1988 as a reference	
1,3-dinitropyrene		075321-20-9					683.15	crude: pyrene + 50 C	
1,6-dinitropyrene		042397-64-8					683.15	crude: pyrene + 50 C	
1,8-dinitropyrene		042397-65-9					683.15	crude: pyrene + 50 C	
2,7-dinitropyrene		117929-15-4					683.15	crude: pyrene + 50 C	
dinitropyrenes (mixed)		078432-19-6					683.15	crude: pyrene + 50 C	
hexachloro-1,3-butadiene		000087-68-3		215	deg C	19; 99	488.15		
4,4'-methylene bis(2-chloroaniline)		000101-14-4		378.9	deg C	83	652.05		
pentachlorophenol		000087-86-5		309.5	deg C	25	582.65	decomposes	
aldrin		000309-00-2		664	deg K	87	664.01	estimated using Clausius Clapyron equation	
dieldrin		000060-57-1		330	deg C	48	603.15	estm'd?; same data given in SRC data set	
p,p'-DDT		000050-29-3		260	deg C	60	533.15	not given in ref 85	
p,p'-DDD		000072-54-8		350	deg C	85	623.15		
p,p'-DDE		000072-55-9		336	deg C	85	609.15		
heptachlor		000076-44-8		310	deg C	85	583.15		
heptachlor epoxide		001024-57-3		no data			583.15	<b>No data available; use value for heptachlor for now</b>	
methoxychlor		000072-43-5		346	deg C	85	619.15	one ref says that it decomposes when heated, so no data...; however SRC data set has 583.15	
mirex		002385-85-5		no data		65	960	<b>hypothetical estm based on Tb vs. Tm regression</b>	
toxaphene		008001-35-2					580	<b>decomposes; hypothetical Tb estimated using Tb vs Tm regression</b>	
endrin		000072-20-8					720	<b>decomposes at 245 deg C when heated, ref 22; estimate for hypothetical Tb</b>	
alpha-hexachlorocyclohexane		000319-84-6		288	deg C	31	561.15		
beta-hexachlorocyclohexane		000319-85-7		301.59	deg C	estm-29-92	574.74	based on 60 deg C @ 0.5 mm Hg	
delta-hexachlorocyclohexane		000319-86-8		312.43	deg C	estm-29-92	585.58	based on 60 deg C @ 0.36 mm Hg	
gamma-hexachlorocyclohexane		000058-89-9		323.4	deg C	31	596.55		
mixed hexachlorocyclohexanes		000319-84-6							

NAME	IUPAC #	cas # (1)	range	average	units	ref	BOILING POINT		notes
							boiling point	boiling point	
cadmium	007440-43-9			767	deg C	71	1040.15		
cadmium carbonate	000513-78-0			no data		71			
cadmium chloride	010108-64-2			960	deg C	71	1233.15		
cadmium oxide	001306-19-0			decomposes at 900 C		71			
cadmium sulfate	010124-36-4			no data		71			
cadmium sulfide	001306-23-6			sublimes in N2 at 980 C		71			
elemental mercury	007439-97-6			356.58	deg C	94	629.73		
mercury oxide	021908-53-2								
mercuric chloride	007487-94-7			302	deg C	94	575.15		
monomethyl mercury chloride	000115-09-3			no data		95	666	hypothetical estm using Tb vs Tm correlation	
dimethyl mercury	000593-74-8								
tetraethyl lead	000078-00-2		200 - 227.2	213.6	deg C	85	486.75		
tetramethyl lead	000075-74-1			274.24	deg C	estm	547.39	based on Bp of 110 deg C at 10 mm Hg, reported in HSDB from IARC volume	
triethyl lead radical (1+ cation)	014570-15-1								
triethyl lead hydride	005224-23-7								
triethyl lead chloride	001067-14-7								
diethyl lead radical (2+ cation)	024952-65-6								
diethyl lead dihydride	081494-11-3								
diethyl lead dichloride	013231-90-8								
trimethyl lead radical (1+ cation)	014570-16-2								
trimethyl lead hydride	007442-13-9								
trimethyl lead chloride	001520-78-1								
dimethyl lead radical (2+ cation)	021774-13-0								
dimethyl lead dihydride	030691-92-0								
dimethyl lead dichloride	001520-77-0								
bis (tributyltin) oxide	000056-35-9			669.14	deg K	estm	669.14	based on 254 deg C at 50 mmHg from ref 97	
tributyl tin	000688-75-3								
tributyltin fluoride	001983-10-4								
tributyltin chloride	001461-22-9								
tributyltin hydroxide	001067-97-6								
tributyltin naphthenate									
tris(tributylstanny) phosphate	013435-05-7								

NAME	BOILING POINT						
					for V/P		
						boiling	
		boiling	boiling	boiling	boiling	point	
		point	point	point	point	point	data
common chemical name	IUPAC #	cas # (1)	range	average	units	ref	deg K
							notes
1,4-dichlorobenzene	000106-46-7		174.6	deg C	5	447.75	
1,2,3,4-tetrachlorobenzene	000634-66-2		254	deg C	5	527.15	similar in Aldrich catalog
1,2,4,5-tetrachlorobenzene	000095-94-3		243	deg C	5	516.15	similar in Aldrich catalog
1,2,3,5-tetrachlorobenzene	000634-90-2		246	deg C	5	519.15	
pentachlorobenzene	000608-93-5		277	deg C	5	550.15	similar in Aldrich catalog
hexachlorobenzene	000118-74-1		322	deg C	5	595.15	similar in Aldrich catalog
naphthalene	000091-20-3		218	deg C	6	491.15	
acenaphthene	000083-32-9		277.5	deg C	6	550.65	
acenaphthylene	000208-96-8	265-275	270	deg C	6	543.15	
fluorene	000086-73-7		295	deg C	6	568.15	
phenanthrene	000085-01-8		339	deg C	6	612.15	
anthracene	000120-12-7		340	deg C	6	613.15	
pyrene	000129-00-0		360	deg C	6	633.15	
floranthene	000206-44-0		375	deg C	6	648.15	
chrysene	000218-01-9		448	deg C	6	721.15	
benz [ a ] anthracene	000056-55-3		435	deg C	6	708.15	
benzo [ b ] fluoranthene	000205-99-2		481	deg C	6	754.15	
benzo [ j ] fluoranthene	000205-82-3		480	deg C	6	753.15	
benzo [ k ] fluoranthene	000207-08-9		481	deg C	6	754.15	
benzo [ a ] pyrene	000050-32-8		495	deg C	6	768.15	
benzo [ e ] pyrene	000192-97-2		561	deg C	79	834.55	Estimated using calculation; value not given in Ref 6; 310-312 deg C at 10 mm
perylene	000198-55-0		495	deg C	6	768.15	
benzo [ g,h,i ] perylene	000191-24-2		550	deg C	11	823.15	
dibenz [ a,h ] anthracene	000053-70-3		524	deg C	6	797.15	
indeno [ 1,2,3-c,d ] pyrene	000193-39-5		530	deg C	11	803.15	

BOILING POINT							
NAME	IUPAC #	cas # (1)	range	average	units	ref	for V/P
							boiling
common chemical name			point	point	point	point	point
			boiling	boiling	boiling	boiling	data
							notes
2,3,7,8-TCDD	001746-01-6			446.5 deg C	6	719.65	
1,2,3,7,8-PeCDD	040321-76-4			464.7 deg C	6	737.85	using value for 12347 PeCDD
1,2,3,4,7,8-HxCDD	039227-28-6			487.7 deg C	6	760.85	
1,2,3,6,7,8-HxCDD	057653-85-7			487.7 deg C	6	760.85	using value for 123478 HxCDD
1,2,3,7,8,9-HxCDD	019408-74-3			487.7 deg C	6	760.85	using value for 123478 HxCDD
1,2,3,4,6,7,8-HpCDD	035822-46-9			507.2 deg C	6	780.35	
OCDD	003268-87-9			510 deg C	6	783.15	
2,3,7,8-TCDF	051207-31-9			438.3 deg C	6	711.45	
2,3,4,7,8-PeCDF	057117-31-4			464.7 deg C	6	737.85	
1,2,3,7,8-PeCDF	057117-41-6			464.7 deg C	6	737.85	using value for 23478 PeCDF
1,2,3,4,7,8-HxCDF	070648-26-9			487.7 deg C	6	760.85	
1,2,3,6,7,8-HxCDF	057117-44-9			487.7 deg C	6	760.85	
1,2,3,7,8,9-HxCDF	072918-21-9			487.7 deg C	6	760.85	using avg of values for 123478 HxCDF and 123678 HxCDF
2,3,4,6,7,8-HxCDF	060851-34-5			487.7 deg C	6	760.85	using avg of values for 123478 HxCDF and 123678 HxCDF
1,2,3,4,6,7,8-HpCDF	067562-39-4			507.2 deg C	6	780.35	
1,2,3,4,7,8,9-HpCDF	055673-89-7			507.2 deg C	6	780.35	
OCDF	039001-02-0			537 deg C	6	810.15	

BOILING POINT							
NAME				for V/P		boiling	
		boiling	boiling	boiling	boiling	point	data
common chemical name	IUPAC #	cas # (1)	range	average	units	ref	deg K
biphenyl	0	000092-52-4		255	deg C	5	528.15
2-PCB	1	002051-60-7		274	deg C	5	547.15
3-PCB	2	002051-61-8		284	deg C	5	557.15
4-PCB	3	002051-62-9		291	deg C	5	564.15
count							
average							
standard deviation							
minimum							
maximum							
2,2'-PCB	4	013029-08-8		not in ref 5		565	estimated using Tb vs Tm regression
2,3-PCB	5	016605-91-7		not in ref 5		508	estimated using Tb vs Tm regression
2,4-PCB	7	033284-50-3		not in ref 5		531	estimated using Tb vs Tm regression
2,4'-PCB	8	034883-43-7		not in ref 5		548	estimated using Tb vs Tm regression
2,5-PCB	9	034883-39-1		not in ref 5		532	estimated using Tb vs Tm regression
2,6-PCB	10	033146-45-1		not in ref 5		541	estimated using Tb vs Tm regression
3,3'-PCB	11	002050-67-1		322	deg C	5	595.15
3,4-PCB	12	002974-92-7		not in ref 5		554	estimated using Tb vs Tm regression
3,5-PCB	14	034883-41-5		not in ref 5		537	estimated using Tb vs Tm regression
4,4'-PCB	15	002050-68-2		315	deg C	5	588.15
count							
average							
standard deviation							
minimum							
maximum							

BOILING POINT							
NAME	IUPAC #	cas # (1)	range	average	units	ref	for V/P
common chemical name			boiling point	boiling point	boiling point	boiling point	boiling point
			range	average	units	ref	data
2,2',3-PCB	16	038444-78-9		<i>not in ref 5</i>		534	estimated using Tb vs Tm regression
2,2',5-PCB	18	037680-65-2		<i>not in ref 5</i>		549	estimated using Tb vs Tm regression
2,3,3'-PCB	20	038444-84-7		<i>not in ref 5</i>		549	estimated using Tb vs Tm regression
2,3,4-PCB	21	055702-46-0		<i>not in ref 5</i>		603	estimated using Tb vs Tm regression
2,3',5-PCB	26	038444-85-8		<i>not in ref 5</i>		546	estimated using Tb vs Tm regression
2,4,4'-PCB	28	007012-37-5		<i>not in ref 5</i>		561	estimated using Tb vs Tm regression
2,4,5-PCB	29	015862-07-4		<i>not in ref 5</i>		581	estimated using Tb vs Tm regression
2,4,6-PCB	30	035693-92-6		<i>not in ref 5</i>		566	estimated using Tb vs Tm regression
2,4',5,-PCB	31	016606-02-3		<i>not in ref 5</i>		571	estimated using Tb vs Tm regression
2',3,4-PCB	33	038444-86-9		<i>not in ref 5</i>		564	estimated using Tb vs Tm regression
3,3',4-PCB	35	037680-69-6		<i>not in ref 5</i>		589	estimated using Tb vs Tm regression
3,4,4'-PCB	37	038444-90-5		<i>not in ref 5</i>		589	estimated using Tb vs Tm regression
count							
average							
standard deviation							
minimum							
maximum							
2,2',3,3'-PCB	40	038444-93-8		<i>not in ref 5</i>		621	estimated using Tb vs Tm regression
2,2',3,5'-PCB	44	041464-39-5		<i>not in ref 5</i>		552	estimated using Tb vs Tm regression
2,2',4,4'-PCB	47	002437-79-8		<i>not in ref 5</i>		585	estimated using Tb vs Tm regression
2,2',4,5'-PCB	49	041464-40-8		<i>not in ref 5</i>		568	estimated using Tb vs Tm regression
2,2',4,6-PCB	50	062796-65-0		<i>not in ref 5</i>		552	estimated using Tb vs Tm regression
2,2',4,6'-PCB	51	068194-04-7		<i>not in ref 5</i>		508	estimated using Tb vs Tm regression
2,2,5,5'-PCB	52	035693-99-3		<i>not in ref 5</i>		589	estimated using Tb vs Tm regression
2,2,5,6'-PCB	53	041464-41-9		<i>not in ref 5</i>		605	estimated using Tb vs Tm regression
2,2,6,6'-PCB	54	015968-05-5		<i>not in ref 5</i>		693	estimated using Tb vs Tm regression
2,3,4,4'-PCB	60	033025-41-1		<i>not in ref 5</i>		640	estimated using Tb vs Tm regression
2,3,4,5-PCB	61	033284-53-6		<i>not in ref 5</i>		594	estimated using Tb vs Tm regression
2,3,5,6-PCB	65	033284-54-7		<i>not in ref 5</i>		582	estimated using Tb vs Tm regression
2,3,4,4'-PCB	66	032598-10-0		<i>not in ref 5</i>		624	estimated using Tb vs Tm regression
2,3',4',5-PCB	70	032598-11-1		<i>not in ref 5</i>		605	estimated using Tb vs Tm regression
2,4,4',6-PCB	75	032598-12-2		<i>not in ref 5</i>		566	estimated using Tb vs Tm regression
3,3',4,4'-PCB	77	032598-13-3		<i>not in ref 5</i>		676	estimated using Tb vs Tm regression
3,3',5,5'-PCB	80	033284-52-5		<i>not in ref 5</i>		661	estimated using Tb vs Tm regression
3,4,4',5-PCB	81	070362-50-4		<i>not in ref 5</i>		659	estimated using Tb vs Tm regression
count							
average							
standard deviation							
minimum							
maximum							

NAME							BOILING POINT					
common chemical name	IUPAC #	cas # (1)	range	average	units	ref	for V/P	boiling	point	point	data	
2,2',3,3',5-PCB	83	060145-20-2		<i>not in ref 5</i>			586	estimated using Tb vs Tm regression				
2,2',3,4,5-PCB	86	065510-45-4		<i>not in ref 5</i>			601	estimated using Tb vs Tm regression				
2,2',3,4,5'-PCB	87	038380-02-8		<i>not in ref 5</i>			614	estimated using Tb vs Tm regression				
2,2',3,4,6-PCB	88	055215-17-3		<i>not in ref 5</i>			601	estimated using Tb vs Tm regression				
2,2',3,5,6-PCB	95	038379-99-6		<i>not in ref 5</i>			601	estimated using Tb vs Tm regression				
2,2',4,4,5-PCB	99	038380-01-7		<i>not in ref 5</i>			564	estimated using Tb vs Tm regression				
2,2',4,4',6-PCB	100	039485-83-1		<i>not in ref 5</i>			508	estimated using Tb vs Tm regression				
2,2',4,5,5'-PCB	101	037680-73-2		<i>not in ref 5</i>			579	estimated using Tb vs Tm regression				
2,2',4,6,6'-PCB	104	056558-16-8		<i>not in ref 5</i>			590	estimated using Tb vs Tm regression				
2,3,3',4,4'-PCB	105	032598-14-4		<i>not in ref 5</i>			606	estimated using Tb vs Tm regression				
2,3,3',4',6-PCB	110	038380-03-9		<i>not in ref 5</i>			558	estimated using Tb vs Tm regression				
2,3,4,4',5-PCB	114	074472-37-0		<i>not in ref 5</i>			612	estimated using Tb vs Tm regression				
2,3,4,5,6-PCB	116	018259-05-7		<i>not in ref 5</i>			624	estimated using Tb vs Tm regression				
2,3',4,4',5-PCB	118	031508-00-6		<i>not in ref 5</i>			608	estimated using Tb vs Tm regression				
2',3,4,5,5'-PCB	124	070424-70-3		<i>not in ref 5</i>			617	estimated using Tb vs Tm regression				
3,3',4,4',5-PCB	126	057465-28-8		<i>not in ref 5</i>			658	estimated using Tb vs Tm regression				
count												
average												
standard deviation												
minimum												
maximum												
2,2',3,3',4,4'-PCB	128	038380-07-3		<i>not in ref 5</i>			648	estimated using Tb vs Tm regression				
2,2',3,3',4,5-PCB	129	055215-18-4		<i>not in ref 5</i>			587	estimated using Tb vs Tm regression				
2,2',3,3',5,6-PCB	134	052704-70-8		<i>not in ref 5</i>			601	estimated using Tb vs Tm regression				
2,2',3,3',6,6'-PCB	136	038411-22-2		<i>not in ref 5</i>			613	estimated using Tb vs Tm regression				
2,2',3,4,4',5'-PCB	138	035065-28-2		<i>not in ref 5</i>			583	estimated using Tb vs Tm regression				
2,2',3,4',5,6-PCB	149	038380-04-0		<i>not in ref 5</i>			581	estimated using Tb vs Tm regression				
2,2',4,4',5,5'-PCB	153	035065-27-1		<i>not in ref 5</i>			604	estimated using Tb vs Tm regression				
2,2',4,4',6,6'-PCB	155	033979-03-2		<i>not in ref 5</i>			614	estimated using Tb vs Tm regression				
2,3,3',4,4',5-PCB	156	038380-08-4		<i>not in ref 5</i>			629	estimated using Tb vs Tm regression				
2,3,3',4,4',5'-PCB	157	069782-90-7		<i>not in ref 5</i>			659	estimated using Tb vs Tm regression				
2,3',4,4',5,5'-PCB	167	052663-72-6		<i>not in ref 5</i>			625	estimated using Tb vs Tm regression				
3,3',4,4',5,5'-PCB	169	032774-16-6		<i>not in ref 5</i>			696	estimated using Tb vs Tm regression				
count												
average												
standard deviation												
minimum												
maximum												

BOILING POINT							
NAME	IUPAC #	cas # (1)	range	average	units	ref	for V/P
							boiling
common chemical name							point
							data
2,2',3,3',4,4',5-PCB	170	035065-30-6		<i>not in ref 5</i>			636   estimated using Tb vs Tm regression
2,2',3,3',4,4',6-PCB	171	052663-71-5		<i>not in ref 5</i>			622   estimated using Tb vs Tm regression
2,2',3,4,4',5,5'-PCB	180	035065-29-3		<i>not in ref 5</i>			611   estimated using Tb vs Tm regression
2,2',3,4,5,5',6-PCB	185	052712-05-7		<i>not in ref 5</i>			647   estimated using Tb vs Tm regression
2,2',3,4',5,5',6-PCB	187	052663-68-0		<i>not in ref 5</i>			605   estimated using Tb vs Tm regression
2,3,3',4,4',5,5'-PCB	189	039635-31-9		<i>not in ref 5</i>			659   estimated using Tb vs Tm regression
count							
average							
standard deviation							
minimum							
maximum							
2,2',3,3',4,4',5,5'-PCB	194	035694-08-7		<i>not in ref 5</i>			656   estimated using Tb vs Tm regression
2,2',3,3',5,5',6,6'-PCB	202	002136-99-4		<i>not in ref 5</i>			659   estimated using Tb vs Tm regression
count							
average							
standard deviation							
minimum							
maximum							
2,2',3,3',4,4',5,5',6-PCB	206	040186-72-9		<i>not in ref 5</i>			700   estimated using Tb vs Tm regression
2,2',3,3',4,4',5,6,6'-PCB	207	052663-79-3		<i>not in ref 5</i>			707   estimated using Tb vs Tm regression
2,2',3,3',4,5,5',6,6'-PCB	208	052663-77-1		<i>not in ref 5</i>			678   estimated using Tb vs Tm regression
count							
average							
standard deviation							
minimum							
maximum							
2,2',3,3',4,4',5,5',6,6'-PCB	209	002051-24-3		<i>not in ref 5</i>			793   estimated using Tb vs Tm regression

VAPOR PRESSURE - solid phase									
NAME		P sub s		for V/P calculation		solid			
common chemical name	IUPAC #	cas # (1)	vapor pressure	at what temp?	units	temp?	units	refer	Vp T(Vp) deg K data notes
octachlorostyrene	029082-74-4		1.32E-005 mm Hg	25	deg C	85	1.7E-008	298.15	SRC data set cites estimate by Neely and Blau, 1985
4-bromophenyl phenyl ether	000101-55-3								
3,3'-dichlorobenzidine	000091-94-1		4.5E-009 mm Hg	20	deg C	ATSDR	5.9E-012	293.15	this is much lower than the value in MacKay's compilation, which came from M
1,3-dinitropyrene	075321-20-9		1.93E-008 mm Hg	25	deg	91	2.5E-011	298.15	estimated: see ref 91
1,6-dinitropyrene	042397-64-8		1.93E-008 mm Hg	25	deg	91	2.5E-011	298.15	estimated: see ref 91
1,8-dinitropyrene	042397-65-9		1.93E-008 mm Hg	25	deg	91	2.5E-011	298.15	estimated: see ref 91
2,7-dinitropyrene	117929-15-4		1.93E-008 mm Hg	25	deg	91	2.5E-011	298.15	estimated: see ref 91
dinitropyrenes (mixed)	078432-19-6		1.93E-008 mm Hg	25	deg	91	2.5E-011	298.15	estimated: see ref 91
hexachloro-1,3-butadiene	000087-68-3								
4,4'-methylene bis(2-chloroaniline)	000101-14-4		1E-005 mm Hg	25	deg C	16	1.3E-008	298.15	data for other temperatures also reported; note that SRC reports a much lower
pentachlorophenol	000087-86-5		0.00415 Pa	25	deg C	8	4.1E-008	298.15	
aldrin	000309-00-2		3.75E-005 mm Hg	20	deg C	49	1.6E-007	298.15	use data from ref 84 for V/P calc; ATSDR much different.
diechlorin	000060-57-1		3.75E-006 mm Hg	20	deg C	49	7.8E-009	298.15	use data from ref 84 for V/P calc; ATSDR much different.
p,p'-DDT	000050-29-3		1.6E-007 mm Hg	20	deg C	85	2.1E-010	293.15	
p,p'-DDD	000072-54-8		6.70E-007 mm Hg	20	deg C	85	8.8E-010	293.15	
p,p'-DDE	000072-55-9		6.0E-006 mm Hg	25	deg C	85	7.9E-009	298.15	
heptachlor	000076-44-8		4E-004 mm Hg	25	deg C	9; 85	5.3E-007	298.15	expt'l
heptachlor epoxide	001024-57-3		1.95E-005 mm Hg	30	deg C	3; 85	2.6E-008	303.15	ref 43 lists as estimated; ref 85 lists as expt'l, and gives reference
methoxychlor	000072-43-5		1.4E-006 mm Hg	25	deg C	25	1.9E-009	298.15	estimated based on EPA P-Chem Program; SRC data set gives a value of 2.5
mirex	002385-85-5		8E-007 mm Hg	25	deg C	85	1.1E-009	298.15	
toxaphene	008001-35-2								
endrin	000072-20-8		3E-006 mm Hg	20	deg C	43	3.9E-009	293.15	
alpha-hexachlorocyclohexane	000319-84-6		4.5E-005 mm Hg	25	deg C	85	5.9E-008	298.15	Schwabe and Legler 1960; extrapolated
beta-hexachlorocyclohexane	000319-85-7		4.66E-007 mm Hg	25	deg C	85	6.1E-010	298.15	Schwabe and Legler 1960; extrapolated
delta-hexachlorocyclohexane	000319-86-8		3.52E-005 mm Hg	25	deg C	85	4.6E-008	298.15	Schwabe and Legler 1960; extrapolated
gamma-hexachlorocyclohexane	000058-89-9		4.0E-008 atm	25	deg C	93	4.0E-008	298.15	see note 93
mixed hexachlorocyclohexanes	000319-84-6								

VAPOR PRESSURE - solid phase									
NAME		P sub s		for V/P calculation					
		solid							
		phase		solid					
common chemical name	IUPAC #	cas # (1)	vapor pressure	at what temp	temp?	Vp atm	T(Vp) deg K	data notes	
cadmium	007440-43-9								
cadmium carbonate	000513-78-0								
cadmium chloride	010108-64-2								
cadmium oxide	001306-19-0		1 mm Hg	1000	deg C	75	1.3E-003	1273.15	
cadmium sulfate	010124-36-4								
cadmium sulfide	001306-23-6								
elemental mercury	007439-97-6								
mercury oxide	021908-53-2								
mercuric chloride	007487-94-7		1 mm Hg	136.2	deg C	94	1.3E-003	409.35	
monomethyl mercury chloride	000115-09-3		0.0085 mm Hg	25	deg C	95	1.1E-005	298.15	note: HSDB gives much higher vapor pressure
dimethyl mercury	000593-74-8								
tetraethyl lead	000078-00-2								
tetramethyl lead	000075-74-1								
triethyl lead radical (1+ cation)	014570-15-1								
triethyl lead hydride	005224-23-7								
triethyl lead chloride	001067-14-7								
diethyl lead radical (2+ cation)	024952-65-6								
diethyl lead dihydride	081494-11-3								
diethyl lead dichloride	013231-90-8								
trimethyl lead radical (1+ cation)	014570-16-2								
trimethyl lead hydride	007442-13-9								
trimethyl lead chloride	001520-78-1								
dimethyl lead radical (2+ cation)	021774-13-0								
dimethyl lead dihydride	030691-92-0								
dimethyl lead dichloride	001520-77-0								
bis (tributyltin) oxide	000056-35-9								
tributyl tin	000688-75-3								
tributyltin fluoride	001983-10-4								
tributyltin chloride	001461-22-9								
tributyltin hydroxide	001067-97-6								
tributyltin naphthenate									
tris(tributylstanny) phosphate	013435-05-7								

VAPOR PRESSURE - solid phase										
NAME	P sub s	for V/P calculation	solid	vapor	at what temp	Vp	T(Vp)			
common chemical name	IUPAC #	cas # (1)	pressure	units	temp?	units	atm	deg K	notes	
1,4-dichlorobenzene	000106-46-7		90.2	Pa	25	deg C	5	8.9E-004	298.15	since a solid at room temp; used saturated Vp for this
1,2,3,4-tetrachlorobenzene	000634-66-2		5.2	Pa	25	deg C	5	5.1E-005	298.15	since a solid at room temp; used saturated Vp for this
1,2,4,5-tetrachlorobenzene	000095-94-3		0.72	Pa	25	deg C	5	7.1E-006	298.15	since a solid at room temp; used saturated Vp for this
1,2,3,5-tetrachlorobenzene	000634-90-2		9.8	Pa	25	deg C	5	9.7E-005	298.15	since a solid at room temp; used saturated Vp for this
pentachlorobenzene	000608-93-5		0.22	Pa	25	deg C	5	2.2E-006	298.15	since a solid at room temp; used saturated Vp for this
hexachlorobenzene	000118-74-1		0.0023	Pa	25	deg C	5	2.3E-008	298.15	since a solid at room temp; used saturated Vp for this
naphthalene	000091-20-3		10.4	Pa	25	deg C	6	1.0E-004	298.15	
acenaphthene	000083-32-9		0.3	Pa	25	deg C	6	3.0E-006	298.15	
acenaphthylene	000208-96-8		0.9	Pa	25	deg C	6	8.9E-006	298.15	
fluorene	000086-73-7		0.09	Pa	25	deg C	6	8.9E-007	298.15	
phenanthrene	000085-01-8		0.02	Pa	25	deg C	6	2.0E-007	298.15	
anthracene	000120-12-7		0.001	Pa	25	deg C	6	9.9E-009	298.15	
pyrene	000129-00-0		0.0006	Pa	25	deg C	6	5.9E-009	298.15	
floranthene	000206-44-0		0.00123	Pa	25	deg C	6	1.2E-008	298.15	
chrysene	000218-01-9		5.7E-007	Pa	25	deg C	6	5.6E-012	298.15	
benz [ a ] anthracene	000056-55-3		3.1E-008	mm Hg	25	deg C	85	4.0E-011	298.15	from SRC data set; a "new" - presumably better - value to use, to see if V/P e
benzo [ b ] fluoranthene	000205-99-2		5.0E-007	mm Hg	25	deg C	80	6.6E-010	298.15	SRC data set
benzo [ j ] fluoranthene	000205-82-3		1.5E-008	mm Hg	25	deg C	81	2.0E-011	298.15	HSDB 1994, cited in ATSDR PAH
benzo [ k ] fluoranthene	000207-08-9		5.2E-008	Pa	25	deg C	6	5.1E-013	298.15	
benzo [ a ] pyrene	000050-32-8		7.0E-007	Pa	25	deg C	6	6.9E-012	298.15	
benzo [ e ] pyrene	000192-97-2		7.4E-007	Pa	25	deg C	6	7.3E-012	298.15	
perylene	000198-55-0		1.4E-008	Pa	25	deg C	6	1.4E-013	298.15	
benzo [ g,h,i ] perylene	000191-24-2		1.0E-010	mm Hg	25	deg C	10	1.4E-013	298.15	ref 10 cited in ATSDR-PAH
dibenz [ a,h ] anthracene	000053-70-3		3.7E-010	Pa	25	deg C	6	3.7E-015	298.15	
indeno [ 1,2,3-c,d ] pyrene	000193-39-5		1.0E-010	mm Hg	20	deg C	82	1.4E-013	293.15	20 deg C; cited in SRC data set

VAPOR PRESSURE - solid phase									
NAME		P sub s for V/P calculation							
		solid		solid					
common chemical name	IUPAC #	cas # (1)	vapor pressure	at what temp	Vp	T(Vp)	data		
			units	temp?	units	refer	atm	deg K	notes
2,3,7,8-TCDD	001746-01-6		7.4E-010 mmHg	25 deg C	78	9.7E-013	298.15	since a solid at room temp; used saturated Vp for this	
1,2,3,7,8-PeCDD	040321-76-4		8.8E-008 Pa	25 deg C	6	8.7E-013	298.15	since a solid at room temp; used saturated Vp for this	
1,2,3,4,7,8-HxCDD	039227-28-6		5.1E-009 Pa	25 deg C	6	5.0E-014	298.15	since a solid at room temp; used saturated Vp for this	
1,2,3,6,7,8-HxCDD	057653-85-7		5.1E-009 Pa	25 deg C	6	5.0E-014	298.15	since a solid at room temp; used saturated Vp for this	
1,2,3,7,8,9-HxCDD	019408-74-3		5.1E-009 Pa	25 deg C	6	5.0E-014	298.15	since a solid at room temp; used saturated Vp for this	
1,2,3,4,6,7,8-HpCDD	035822-46-9		7.5E-010 Pa	25 deg C	6	7.4E-015	298.15	since a solid at room temp; used saturated Vp for this	
OCDD	003268-87-9		1.1E-010 Pa	25 deg C	6	1.1E-015	298.15	since a solid at room temp; used saturated Vp for this	
2,3,7,8-TCDF	051207-31-9		2.0E-006 Pa	25 deg C	6	2.0E-011	298.15	since a solid at room temp; used saturated Vp for this	
2,3,4,7,8-PeCDF	057117-31-4		3.5E-007 Pa	25 deg C	6	3.5E-012	298.15	since a solid at room temp; used saturated Vp for this	
1,2,3,7,8-PeCDF	057117-41-6		3.5E-007 Pa	25 deg C	6	3.5E-012	298.15	since a solid at room temp; used saturated Vp for this	
1,2,3,4,7,8-HxCDF	070648-26-9		3.2E-008 Pa	25 deg C	6	3.2E-013	298.15	since a solid at room temp; used saturated Vp for this	
1,2,3,6,7,8-HxCDF	057117-44-9		3.5E-008 Pa	25 deg C	6	3.5E-013	298.15	since a solid at room temp; used saturated Vp for this	
1,2,3,7,8,9-HxCDF	072918-21-9		3.35E-008 Pa	25 deg C	6	3.3E-013	298.15	since a solid at room temp; used saturated Vp for this	
2,3,4,6,7,8-HxCDF	060851-34-5		3.35E-008 Pa	25 deg C	6	3.3E-013	298.15	since a solid at room temp; used saturated Vp for this	
1,2,3,4,6,7,8-HpCDF	067562-39-4		4.7E-009 Pa	25 deg C	6	4.6E-014	298.15	since a solid at room temp; used saturated Vp for this	
1,2,3,4,7,8,9-HpCDF	055673-89-7		6.2E-009 Pa	25 deg C	6	6.1E-014	298.15	since a solid at room temp; used saturated Vp for this	
OCDF	039001-02-0		5.0E-010 Pa	25 deg C	6	4.9E-015	298.15	since a solid at room temp; used saturated Vp for this	

VAPOR PRESSURE - solid phase							
		P sub s		for V/P calculation			
		solid		solid			
NAME		vapor	at what temp	Vp	T(Vp)	data	
common chemical name	IUPAC #	cas # (1)	pressure	units	temp?	units	refer
biphenyl	0	000092-52-4	1.3	Pa	25	deg C	5
2-PCB	1	002051-60-7	2.04	Pa	25	deg C	5
3-PCB	2	002051-61-8	1	Pa	25	deg C	5
4-PCB	3	002051-62-9	0.279	Pa	25	deg C	5
count							
average							
standard deviation							
minimum							
maximum							
2,2'-PCB	4	013029-08-8	0.265	Pa	25	deg C	5
2,3-PCB	5	016605-91-7	<i>not in ref 5; see liquid estm at right</i>				
2,4-PCB	7	033284-50-3	0.254	Pa	25	deg C	5
2,4'-PCB	8	034883-43-7	2.09E-003	mm Hg	25	deg C	85
2,5-PCB	9	034883-39-1	0.18	Pa	25	deg C	5
2,6-PCB	10	033146-45-1	1.91E-004	mm Hg	25	deg C	85
3,3'-PCB	11	002050-67-1	0.027	Pa	25	deg C	5
3,4-PCB	12	002974-92-7	1.91E-004	mm Hg	25	deg C	85
3,5-PCB	14	034883-41-5	0.105	Pa	25	deg C	5
4,4'-PCB	15	002050-68-2	0.0048	Pa	25	deg C	5
count							
average							
standard deviation							
minimum							
maximum							

VAPOR PRESSURE - solid phase									
NAME		P sub s		for V/P calculation					
		solid							
		vapor		at what temp		Vp		T(Vp)	
common chemical name	IUPAC #	cas # (1)	pressure	units	temp?	units	refer	atm	deg K
2,2',3-PCB	16	038444-78-9	<i>not in ref 5 or 85</i>						
2,2',5-PCB	18	037680-65-2	0.143	Pa	25	deg C	5		
2,3,3'-PCB	20	038444-84-7	4E-005	mm Hg	25	deg C	85	5.3E-008	298.15
2,3,4-PCB	21	055702-46-0	4E-005	mm Hg	25	deg C	85	5.3E-008	298.15
2,3',5-PCB	26	038444-85-8	<i>not in ref 5 or 85</i>						
2,4,4'-PCB	28	007012-37-5	1.95E-004	mm Hg	25	deg C	85	2.6E-007	298.15
2,4,5-PCB	29	015862-07-4	0.132	Pa	25	deg C	5		
2,4,6-PCB	30	035693-92-6	0.0384	Pa	25	deg C	5		
2,4',5,-PCB	31	016606-02-3	<i>not in ref 5 or 85</i>						
2',3,4-PCB	33	038444-86-9	0.0136	Pa	25	deg C	5		
3,3',4-PCB	35	037680-69-6	<i>not in ref 5 or 85</i>						
3,4,4'-PCB	37	038444-90-5	<i>not in ref 5 or 85</i>						
count									
average									
standard deviation									
minimum									
maximum									
2,2',3,3'-PCB	40	038444-93-8	0.00225	Pa	25	deg C	5		
2,2',3,5'-PCB	44	041464-39-5	8.45E-006	mm Hg	25	deg C	85	1.1E-008	298.15
2,2',4,4'-PCB	47	002437-79-8	0.0054	Pa	25	deg C	5		
2,2',4,5'-PCB	49	041464-40-8	8.48E-006	mm Hg	25	deg C	85	1.1E-008	298.15
2,2',4,6-PCB	50	062796-65-0	8.45E-006	mm Hg	25	deg C	85	1.1E-008	298.15
2,2',4,6'-PCB	51	068194-04-7	<i>not in ref 5; a liquid at room temp</i>						
2,2,5,5'-PCB	52	035693-99-3	0.0049	Pa	25	deg C	5		
2,2,5,6'-PCB	53	041464-41-9	2.05E-004	mm Hg	25	deg C	85	2.7E-007	298.15
2,2,6,6'-PCB	54	015968-05-5	8.45E-006	mm Hg	25	deg C	85	1.1E-008	298.15
2,3,4,4'-PCB	60	033025-41-1	8.45E-006	mm Hg	25	deg C	85	1.1E-008	298.15
2,3,4,5-PCB	61	033284-53-6	3.75E-005	mm Hg	25	deg C	85	4.9E-008	298.15
2,3,5,6-PCB	65	033284-54-7	<i>not in ref 5 or 85</i>						
2,3,4,4'-PCB	66	032598-10-0	8.45E-006	mm Hg	25	deg C	85	1.1E-008	298.15
2,3',4',5-PCB	70	032598-11-1	4.08E-005	mm Hg	25	deg C	85	5.4E-008	298.15
2,4,4',6-PCB	75	032598-12-2	<i>not in ref 5 or 85</i>						
3,3',4,4'-PCB	77	032598-13-3	0.0000588	Pa	25	deg C	5		
3,3',5,5'-PCB	80	033284-52-5	8.45E-006	mm Hg	25	deg C	85	1.1E-008	298.15
3,4,4',5-PCB	81	070362-50-4	<i>not in ref 5 or 85</i>						
count									
average									
standard deviation									
minimum									
maximum									

VAPOR PRESSURE - solid phase									
NAME		P sub s		for V/P calculation					
		solid							
		phase		solid					
common chemical name	IUPAC #	cas # (1)	vapor pressure	at what temp	temp?	Vp atm	T(Vp) deg K	data notes	
2,2',3,3',5-PCB	83	060145-20-2	<i>not in ref 5 or 85</i>						
2,2',3,4,5-PCB	86	065510-45-4	0.00927	Pa	25	deg C 5			
2,2',3,4,5'-PCB	87	038380-02-8	0.000304	Pa	25	deg C 5			
2,2',3,4,6-PCB	88	055215-17-3	2.22E-006	mm Hg	25	deg C 85	2.9E-009	298.15	
2,2',3,5,6-PCB	95	038379-99-6	<i>not in ref 5 or 85</i>						
2,2',4,4,5-PCB	99	038380-01-7	2.2E-005	mm Hg	25	deg C 85	2.9E-008	298.15	
2,2',4,4',6-PCB	100	039485-83-1	liquid at room temperature						
2,2',4,5,5'-PCB	101	037680-73-2	0.00109	Pa	25	deg C 5			
2,2',4,6,6'-PCB	104	056558-16-8	<i>not in ref 5 or 85</i>						
2,3,3',4,4'-PCB	105	032598-14-4	6.53E-006	mm Hg	25	deg C 85	8.6E-009	298.15	
2,3,3',4,6-PCB	110	038380-03-9	2.22E-006	mm Hg	25	deg C 85	2.9E-009	298.15	
2,3,4,4',5-PCB	114	074472-37-0	<i>not in ref 5 or 85</i>						
2,3,4,5,6-PCB	116	018259-05-7	2.22E-006	mm Hg	25	deg C 85	2.9E-009	298.15	
2,3',4,4',5-PCB	118	031508-00-6	<i>not in ref 5 or 85</i>						
2,3,4,5,5'-PCB	124	070424-70-3	<i>not in ref 5 or 85</i>						
3,3',4,4',5-PCB	126	057465-28-8	<i>not in ref 5 or 85</i>						
count									
average									
standard deviation									
minimum									
maximum									
2,2',3,3',4,4'-PCB	128	038380-07-3	0.0000198	Pa	25	deg C 5			
2,2',3,3',4,5-PCB	129	055215-18-4	5.81E-007	mm Hg	25	deg C 85	7.6E-010	298.15	
2,2',3,3',5,6-PCB	134	052704-70-8	1.10E-006	mm Hg	25	deg C 85	1.4E-009	298.15	
2,2',3,3',6,6'-PCB	136	038411-22-2	5.81E-007	mm Hg	25	deg C 85	7.6E-010	298.15	
2,2',3,4,4',5'-PCB	138	035065-28-2	3.79E-006	mm Hg	25	deg C 85	5.0E-009	298.15	
2,2',3,4',5,6-PCB	149	038380-04-0	8.43E-006	mm Hg	25	deg C 85	1.1E-008	298.15	
2,2',4,4',5,5'-PCB	153	035065-27-1	0.000119	Pa	25	deg C 5			
2,2',4,4',6,6'-PCB	155	033979-03-2	0.00048	Pa	25	deg C 5			
2,3,3',4,4',5-PCB	156	038380-08-4	1.61E-006	mm Hg	25	deg C 85	2.1E-009	298.15	
2,3,3',4,4',5'-PCB	157	069782-90-7	<i>not in ref 5 or 85</i>						
2,3',4,4',5,5'-PCB	167	052663-72-6	5.81E-007	mm Hg	25	deg C 85	7.6E-010	298.15	
3,3',4,4',5,5'-PCB	169	032774-16-6	5.81E-007	mm Hg	25	deg C 85	7.6E-010	298.15	
count									
average									
standard deviation									
minimum									
maximum									

VAPOR PRESSURE - solid phase							
		P sub s		for V/P calculation			
NAME		solid		solid			
common chemical name	IUPAC #	cas # (1)	vapor pressure	at what temp?	Vp	T(Vp)	data
			units	temp?	units	deg K	notes
2,2',3,3',4,4',5-PCB	170	035065-30-6	6.28E-007 mm Hg	25 deg C	85	8.3E-010	298.15
2,2',3,3',4,4',6-PCB	171	052663-71-5	0.0000273 Pa	25 deg C	5		
2,2',3,4,4',5,5'-PCB	180	035065-29-3	9.77E-007 mm Hg	25 deg C	85	1.3E-009	298.15
2,2',3,4,5,5',6-PCB	185	052712-05-7	1.3E-007 mm Hg	25 deg C	85	1.7E-010	298.15
2,2',3,4',5,5',6-PCB	187	052663-68-0	1.3E-007 mm Hg	25 deg C	85	1.7E-010	298.15
2,3,3',4,4',5,5'-PCB	189	039635-31-9	not in ref 5 or 85				
count							
average							
standard deviation							
minimum							
maximum							
2,2',3,3',4,4',5,5'-PCB	194	035694-08-7	2.87E-008 mm Hg	25 deg C	85	3.8E-011	298.15
2,2',3,3',5,5',6,6'-PCB	202	002136-99-4	0.0000266 Pa	25 deg C	5		
count							
average							
standard deviation							
minimum							
maximum							
2,2',3,3',4,4',5,5',6-PCB	206	040186-72-9	1.96E-007 Pa	25 deg C	5		
2,2',3,3',4,4',5,6,6'-PCB	207	052663-79-3	not in ref 5 or 85				
2,2',3,3',4,5,5',6,6'-PCB	208	052663-77-1	7.6E-009 mm Hg	25 deg C	85	1.0E-011	298.15
count							
average							
standard deviation							
minimum							
maximum							
2,2',3,3',4,4',5,5',6,6'-PCB	209	002051-24-3	5.02E-008 Pa	25 deg C	5		

Vapor Pressure Estimation for						
NAME	PCB's Using Correlation of Falconer and Bidleman, 1994					
				liq Vp		
				at temp =		
				298.15		
				deg K		
common chemical name	IUPAC #	cas # (1)	-mL	bl	Pa	NOTES
octachlorostyrene	029082-74-4					
4-bromophenyl phenyl ether	000101-55-3					
3,3'-dichlorobenzidine	000091-94-1					
1,3-dinitropyrene	075321-20-9					
1,6-dinitropyrene	042397-64-8					
1,8-dinitropyrene	042397-65-9					
2,7-dinitropyrene	117929-15-4					
dinitropyrenes (mixed)	078432-19-6					
hexachloro-1,3-butadiene	000087-68-3					
4,4'-methylene bis(2-chloroaniline)	000101-14-4					
pentachlorophenol	000087-86-5					
aldrin	000309-00-2					
dielectron	000060-57-1					
p,p'-DDT	000050-29-3					
p,p'-DDD	000072-54-8					
p,p'-DDE	000072-55-9					
heptachlor	000076-44-8					
heptachlor epoxide	001024-57-3					
methoxychlor	000072-43-5					
mirex	002385-85-5					
toxaphene	008001-35-2					
endrin	000072-20-8					
alpha-hexachlorocyclohexane	000319-84-6					
beta-hexachlorocyclohexane	000319-85-7					
delta-hexachlorocyclohexane	000319-86-8					
gamma-hexachlorocyclohexane	000058-89-9					
mixed hexachlorocyclohexanes	000319-84-6					

Vapor Pressure Estimation for						
NAME	PCB's Using Correlation of Falconer and Bidleman, 1994					
				liq Vp		
				at temp =		
				298.15		
				deg K		
common chemical name	IUPAC #	cas # (1)	-mL	bl	Pa	NOTES
cadmium	007440-43-9					
cadmium carbonate	000513-78-0					
cadmium chloride	010108-64-2					
cadmium oxide	001306-19-0					
cadmium sulfate	010124-36-4					
cadmium sulfide	001306-23-6					
elemental mercury	007439-97-6					
mercury oxide	021908-53-2					
mercuric chloride	007487-94-7					
monomethyl mercury chloride	000115-09-3					
dimethyl mercury	000593-74-8					
tetraethyl lead	000078-00-2					
tetramethyl lead	000075-74-1					
triethyl lead radical (1+ cation)	014570-15-1					
triethyl lead hydride	005224-23-7					
triethyl lead chloride	001067-14-7					
diethyl lead radical (2+ cation)	024952-65-6					
diethyl lead dihydride	081494-11-3					
diethyl lead dichloride	013231-90-8					
trimethyl lead radical (1+ cation)	014570-16-2					
trimethyl lead hydride	007442-13-9					
trimethyl lead chloride	001520-78-1					
dimethyl lead radical (2+ cation)	021774-13-0					
dimethyl lead dihydride	030691-92-0					
dimethyl lead dichloride	001520-77-0					
bis (tributyltin) oxide	000056-35-9					
tributyl tin	000688-75-3					
tributyltin fluoride	001983-10-4					
tributyltin chloride	001461-22-9					
tributyltin hydroxide	001067-97-6					
tributyltin naphthenate						
tris(tributylstanny) phosphate	013435-05-7					

Vapor Pressure Estimation for						
NAME	PCB's Using Correlation of Falconer and Bidleman, 1994					
			liq Vp			
			at temp =			
			298.15			
			deg K			
common chemical name	IUPAC #	cas # (1)	-mL	bl	Pa	NOTES
1,4-dichlorobenzene	000106-46-7					
1,2,3,4-tetrachlorobenzene	000634-66-2					
1,2,4,5-tetrachlorobenzene	000095-94-3					
1,2,3,5-tetrachlorobenzene	000634-90-2					
pentachlorobenzene	000608-93-5					
hexachlorobenzene	000118-74-1					
naphthalene	000091-20-3					
acenaphthene	000083-32-9					
acenaphthylene	000208-96-8					
fluorene	000086-73-7					
phenanthrene	000085-01-8					
anthracene	000120-12-7					
pyrene	000129-00-0					
floranthene	000206-44-0					
chrysene	000218-01-9					
benz [ a ] anthracene	000056-55-3					
benzo [ b ] fluoranthene	000205-99-2					
benzo [ j ] fluoranthene	000205-82-3					
benzo [ k ] fluoranthene	000207-08-9					
benzo [ a ] pyrene	000050-32-8					
benzo [ e ] pyrene	000192-97-2					
perylene	000198-55-0					
benzo [ g,h,i ] perylene	000191-24-2					
dibenz [ a,h ] anthracene	000053-70-3					
indeno [ 1,2,3-c,d ] pyrene	000193-39-5					

			Vapor Pressure Estimation for	
<b>NAME</b>			PCB's Using Correlation of	
			Falconer and Bidleman, 1994	
			liq Vp	
			at temp =	
			298.15	
			deg K	
common chemical name	IUPAC #	cas # (1)	-mL	bl
			Pa	NOTES
2,3,7,8-TCDD	001746-01-6			
1,2,3,7,8-PeCDD	040321-76-4			
1,2,3,4,7,8-HxCDD	039227-28-6			
1,2,3,6,7,8-HxCDD	057653-85-7			
1,2,3,7,8,9-HxCDD	019408-74-3			
1,2,3,4,6,7,8-HpCDD	035822-46-9			
OCDD	003268-87-9			
2,3,7,8-TCDF	051207-31-9			
2,3,4,7,8-PeCDF	057117-31-4			
1,2,3,7,8-PeCDF	057117-41-6			
1,2,3,4,7,8-HxCDF	070648-26-9			
1,2,3,6,7,8-HxCDF	057117-44-9			
1,2,3,7,8,9-HxCDF	072918-21-9			
2,3,4,6,7,8-HxCDF	060851-34-5			
1,2,3,4,6,7,8-HpCDF	067562-39-4			
1,2,3,4,7,8,9-HpCDF	055673-89-7			
OCDF	039001-02-0			

Vapor Pressure Estimation for						
NAME	PCB's Using Correlation of Falconer and Bidleman, 1994					
			liq Vp			
			at temp =			
			298.15			
			deg K			
common chemical name	IUPAC #	cas # (1)	-mL	bl	Pa	NOTES
biphenyl	0	000092-52-4				
2-PCB	1	002051-60-7	3366	11.57	1.9E+000	
3-PCB	2	002051-61-8	3476	11.65	9.8E-001	
4-PCB	3	002051-62-9	3488	11.67	9.4E-001	
count						
average						
standard deviation						
minimum						
maximum						
2,2'-PCB	4	013029-08-8	3642	11.73	3.3E-001	
2,3-PCB	5	016605-91-7	3769	11.81	1.5E-001	
2,4-PCB	7	033284-50-3	3841	12.15	1.9E-001	
2,4'-PCB	8	034883-43-7	3769	11.84	1.6E-001	
2,5-PCB	9	034883-39-1	3862	12.22	1.8E-001	
2,6-PCB	10	033146-45-1	3642	11.74	3.3E-001	
3,3'-PCB	11	002050-67-1	3936	12.14	8.7E-002	
3,4-PCB	12	002974-92-7	3885	11.92	7.8E-002	
3,5-PCB	14	034883-41-5	3885	12.13	1.3E-001	
4,4'-PCB	15	002050-68-2	3971	12.18	7.3E-002	
count						
average						
standard deviation						
minimum						
maximum						

Vapor Pressure Estimation for						
NAME	PCB's Using Correlation of Falconer and Bidleman, 1994					
			liq Vp			
			at temp =			
			298.15			
			deg K			
common chemical name	IUPAC #	cas # (1)	-mL	bl	Pa	NOTES
2,2',3-PCB	16	038444-78-9	3935	11.93	5.4E-002	
2,2',5-PCB	18	037680-65-2	3935	12.09	7.8E-002	
2,3,3'-PCB	20	038444-84-7	4075	12.12	2.8E-002	
2,3,4-PCB	21	055702-46-0	4075	12.11	2.8E-002	
2,3',5-PCB	26	038444-85-8	4075	12.28	4.1E-002	
2,4,4'-PCB	28	007012-37-5	4075	12.2	3.4E-002	
2,4,5-PCB	29	015862-07-4	4007	12.09	4.5E-002	
2,4,6-PCB	30	035693-92-6	3886	12.02	9.7E-002	
2,4',5,-PCB	31	016606-02-3	4058	12.05	2.8E-002	
2',3,4-PCB	33	038444-86-9	4075	12.09	2.6E-002	
3,3',4-PCB	35	037680-69-6	4242	12.37	1.4E-002	
3,4,4'-PCB	37	038444-90-5	4242	12.33	1.3E-002	
count						
average						
standard deviation						
minimum						
maximum						
2,2',3,3'-PCB	40	038444-93-8	4271	12.32	9.9E-003	
2,2',3,5'-PCB	44	041464-39-5	4229	12.29	1.3E-002	
2,2',4,4'-PCB	47	002437-79-8	4229	12.37	1.5E-002	
2,2',4,5'-PCB	49	041464-40-8	4229	12.41	1.7E-002	
2,2',4,6-PCB	50	062796-65-0	not given by Falconer & Bidleman			
2,2',4,6'-PCB	51	068194-04-7	4117	12.2	2.5E-002	
2,2,5,5'-PCB	52	035693-99-3	4220	12.36	1.6E-002	
2,2,5,6'-PCB	53	041464-41-9	4114	12.24	2.8E-002	
2,2,6,6'-PCB	54	015968-05-5	3751	11.17	3.9E-002	
2,3,4,4'-PCB	60	033025-41-1	4382	12.42	5.3E-003	
2,3,4,5-PCB	61	033284-53-6	4382	12.78	1.2E-002	
2,3,5,6-PCB	65	033284-54-7	4229	12.33	1.4E-002	
2,3,4,4'-PCB	66	032598-10-0	4349	12.38	6.2E-003	
2,3',4',5-PCB	70	032598-11-1	4431	12.6	5.5E-003	
2,4,4',6-PCB	75	032598-12-2	4229	12.44	1.8E-002	
3,3',4,4'-PCB	77	032598-13-3	4552	12.61	2.2E-003	
3,3',5,5'-PCB	80	033284-52-5	4598	13.16	5.5E-003	
3,4,4',5-PCB	81	070362-50-4	4598	12.88	2.9E-003	
count						
average						
standard deviation						
minimum						
maximum						

Vapor Pressure Estimation for						
NAME	PCB's Using Correlation of Falconer and Bidleman, 1994					
			liq Vp			
			at temp =			
			298.15			
			deg K			
common chemical name	IUPAC #	cas # (1)	-mL	bl	Pa	NOTES
2,2',3,3',5-PCB	83	060145-20-2	4522	12.6	2.7E-003	
2,2',3,4,5-PCB	86	065510-45-4	4522	12.61	2.8E-003	
2,2',3,4,5'-PCB	87	038380-02-8	4562	12.66	2.3E-003	
2,2',3,4,6-PCB	88	055215-17-3	4399	12.53	6.0E-003	
2,2',3,5,6-PCB	95	038379-99-6	4399	12.48	5.3E-003	
2,2',4,4,5-PCB	99	038380-01-7	4533	12.68	3.0E-003	
2,2',4,4,6-PCB	100	039485-83-1	<b>not given by Falconer &amp; Bidleman</b>			
2,2',4,5,5'-PCB	101	037680-73-2	4514	12.67	3.4E-003	
2,2',4,6,6'-PCB	104	056558-16-8	4522	12.6	2.7E-003	use coefficients for IUPAC #83, which has a similar melting point
2,3,3',4,4'-PCB	105	032598-14-4	4758	12.9	8.7E-004	
2,3,3',4,6-PCB	110	038380-03-9	4522	12.43	1.8E-003	
2,3,4,4',5-PCB	114	074472-37-0	4688	12.82	1.2E-003	
2,3,4,5,6-PCB	116	018259-05-7	4522	12.53	2.3E-003	
2,3',4,4',5-PCB	118	031508-00-6	4664	12.72	1.2E-003	
2',3,4,5,5'-PCB	124	070424-70-3	4688	12.62	7.9E-004	
3,3',4,4',5-PCB	126	057465-28-8	4956	13.31	4.9E-004	
count						
average						
standard deviation						
minimum						
maximum						
2,2',3,3',4,4'-PCB	128	038380-07-3	4881	12.91	3.5E-004	
2,2',3,3',4,5-PCB	129	055215-18-4	4816	12.8	4.4E-004	
2,2',3,3',5,6-PCB	134	052704-70-8	4681	12.79	1.2E-003	
2,2',3,3',6,6'-PCB	136	038411-22-2	4303	11.63	1.6E-003	
2,2',3,4,4',5'-PCB	138	035065-28-2	4800	12.81	5.1E-004	
2,2',3,4',5,6-PCB	149	038380-04-0	4689	12.78	1.1E-003	
2,2',4,4',5,5'-PCB	153	035065-27-1	4775	12.85	6.8E-004	
2,2',4,4',6,6'-PCB	155	033979-03-2	4303	12.02	3.9E-003	
2,3,3',4,4',5-PCB	156	038380-08-4	4949	12.94	2.2E-004	
2,3,3',4,4',5'-PCB	157	069782-90-7	4994	13.05	2.0E-004	
2,3',4,4',5,5'-PCB	167	052663-72-6	4994	13.2	2.8E-004	
3,3',4,4',5,5'-PCB	169	032774-16-6	5313	13.64	6.6E-005	
count						
average						
standard deviation						
minimum						
maximum						

			Vapor Pressure Estimation for			
<b>NAME</b>			PCB's Using Correlation of			
			Falconer and Bidleman, 1994			
				liq Vp		
				at temp =		
				<b>298.15</b>		
				deg K		
common chemical name	IUPAC #	cas # (1)	-mL	bl	Pa	NOTES
2,2',3,3',4,4',5-PCB	170	035065-30-6	5139	13.17	8.6E-005	
2,2',3,3',4,4',6-PCB	171	052663-71-5	5008	13.07	1.9E-004	
2,2',3,4,4',5,5'-PCB	180	035065-29-3	5042	13.03	1.3E-004	
2,2',3,4,5,5',6-PCB	185	052712-05-7	4962	13.15	3.2E-004	
2,2',3,4',5,5',6-PCB	187	052663-68-0	4911	12.96	3.1E-004	
2,3,3',4,4',5,5'-PCB	189	039635-31-9	5300	13.46	4.8E-005	
count						
average						
standard deviation						
minimum						
maximum						
2,2',3,3',4,4',5,5'-PCB	194	035694-08-7	5402	13.43	2.0E-005	
2,2',3,3',5,5',6,6'-PCB	202	002136-99-4	4851	12.99	5.2E-004	
count						
average						
standard deviation						
minimum						
maximum						
2,2',3,3',4,4',5,5',6-PCB	206	040186-72-9	5526	13.57	1.1E-005	
2,2',3,3',4,4',5,6,6'-PCB	207	052663-79-3	5127	12.7	3.2E-005	
2,2',3,3',4,5,5',6,6'-PCB	208	052663-77-1	5127	12.68	3.0E-005	
count						
average						
standard deviation						
minimum						
maximum						
2,2',3,3',4,4',5,5',6,6'-PCB	209	002051-24-3	5402	13.27	1.4E-005	

NAME							VAPOR PRESSURE - liquid phase			
							for V/P calculation			
		liquid			liquid					
		phase			phase					
		vapor	at what temp		Vp	T(Vp)	data			
common chemical name	IUPAC #	cas # (1)	pressure	units	temp?	units	referenc	atm	deg K	notes
octachlorostyrene		029082-74-4								
4-bromophenyl phenyl ether		000101-55-3	0.2 Pa	25 deg C	7	2.0E-006	298.15			
3,3'-dichlorobenzidine		000091-94-1	6.41E-004 Pa	25 deg C	8					
1,3-dinitropyrene		075321-20-9								
1,6-dinitropyrene		042397-64-8								
1,8-dinitropyrene		042397-65-9								
2,7-dinitropyrene		117929-15-4								
dinitropyrenes (mixed)		078432-19-6								
hexachloro-1,3-butadiene		000087-68-3	20 Pa	25 deg C	7	2.0E-004	298.15			ref 99 gives same
4,4'-methylene bis(2-chloroaniline)		000101-14-4								
pentachlorophenol		000087-86-5	0.12 Pa	25 deg C	8					
aldrin		000309-00-2								
die�din		000060-57-1								
p,p'-DDT		000050-29-3								
p,p'-DDD		000072-54-8								
p,p'-DDE		000072-55-9								
heptachlor		000076-44-8								
heptachlor epoxide		001024-57-3								
methoxychlor		000072-43-5								
mirex		002385-85-5								
toxaphene		008001-35-2	6.69E-006 mm Hg	25 deg C	57	8.8E-009	298.15	Murphy paper says that its a subcooled liquid value...		
endrin		000072-20-8								
alpha-hexachlorocyclohexane		000319-84-6								
beta-hexachlorocyclohexane		000319-85-7								
delta-hexachlorocyclohexane		000319-86-8								
gamma-hexachlorocyclohexane		000058-89-9								
mixed hexachlorocyclohexanes		000319-84-6								

VAPOR PRESSURE - liquid phase						
				for V/P calculation		
NAME		liquid		liquid		
common chemical name	IUPAC #	cas # (1)	vapor pressure	at what temp	Vp	T(Vp)
			units	temp <sup>1</sup> units	atm	deg K
cadmium	007440-43-9		1 mm Hg	394 deg C	75, 94	1.3E-003 667.15
cadmium carbonate	000513-78-0					
cadmium chloride	010108-64-2		10 mm Hg	656 deg C	75, 94	1.3E-002 929.15
cadmium oxide	001306-19-0					
cadmium sulfate	010124-36-4					
cadmium sulfide	001306-23-6					
elemental mercury	007439-97-6	0.001201	mm Hg	20 deg C	94	1.6E-006 293.15
mercury oxide	021908-53-2					
mercuric chloride	007487-94-7					
monomethyl mercury chloride	000115-09-3					
dimethyl mercury	000593-74-8					
tetraethyl lead	000078-00-2	3.9E-001	mm Hg	25 deg C	85	5.1E-004 298.15
tetramethyl lead	000075-74-1	22.5	mm Hg	20 deg C	97	3.0E-002 293.15
triethyl lead radical (1+ cation)	014570-15-1					
triethyl lead hydride	005224-23-7					
triethyl lead chloride	001067-14-7					
diethyl lead radical (2+ cation)	024952-65-6					
diethyl lead dihydride	081494-11-3					
diethyl lead dichloride	013231-90-8					
trimethyl lead radical (1+ cation)	014570-16-2					
trimethyl lead hydride	007442-13-9					
trimethyl lead chloride	001520-78-1					
dimethyl lead radical (2+ cation)	021774-13-0					
dimethyl lead dihydride	030691-92-0					
dimethyl lead dichloride	001520-77-0					
bis (tributyltin) oxide	000056-35-9	6.4E-007	mm Hg	20 deg C	97 (atm)	8.4E-010 293.15
tributyl tin	000688-75-3					
tributyltin fluoride	001983-10-4					
tributyltin chloride	001461-22-9					
tributyltin hydroxide	001067-97-6					
tributyltin naphthenate						
tris(tributylstanny) phosphate	013435-05-7					

NAME							VAPOR PRESSURE - liquid phase			
common chemical name	IUPAC #	cas # (1)	liquid	phase	vapor	at what temp	for V/P calculation		data	
							Vp	T(Vp)		
			atm	deg C	Pa	units	atm	deg K	notes	
1,4-dichlorobenzene	000106-46-7		170.19	Pa	25	deg C	5			
1,2,3,4-tetrachlorobenzene	000634-66-2		8.67	Pa	25	deg C	5			
1,2,4,5-tetrachlorobenzene	000095-94-3		9.6	Pa	25	deg C	5			
1,2,3,5-tetrachlorobenzene	000634-90-2		19.22	Pa	25	deg C	5			
pentachlorobenzene	000608-93-5		0.9565	Pa	25	deg C	5			
hexachlorobenzene	000118-74-1		0.2447	Pa	25	deg C	5			
naphthalene	000091-20-3		36.81	Pa	25	deg C	6			
acenaphthene	000083-32-9		1.52	Pa	25	deg C	6			
acenaphthylene	000208-96-8		4.14	Pa	25	deg C	6			
fluorene	000086-73-7		0.715	Pa	25	deg C	6			
phenanthrene	000085-01-8		0.113	Pa	25	deg C	6			
anthracene	000120-12-7		0.0778	Pa	25	deg C	6			
pyrene	000129-00-0		0.0119	Pa	25	deg C	6			
floranthene	000206-44-0		8.72E-003	Pa	25	deg C	6			
chrysene	000218-01-9		1.07E-004	Pa	25	deg C	6			
benz [ a ] anthracene	000056-55-3		6.06E-004	Pa	25	deg C	6			
benzo [ b ] fluoranthene	000205-99-2		<i>not given in reference</i>		6					
benzo [ j ] fluoranthene	000205-82-3		<i>not given in reference</i>		6					
benzo [ k ] fluoranthene	000207-08-9		4.12E-006	Pa	25	deg C	6			
benzo [ a ] pyrene	000050-32-8		2.13E-005	Pa	25	deg C	6			
benzo [ e ] pyrene	000192-97-2		2.41E-005	Pa	25	deg C	6			
perylene	000198-55-0		<i>not given in reference</i>		6					
benzo [ g,h,i ] perylene	000191-24-2		2.25E-005	Pa	25	deg C	6			
dibenz [ a,h ] anthracene	000053-70-3		9.16E-008	Pa	25	deg C	6			
indeno [ 1,2,3-c,d ] pyrene	000193-39-5		<i>not given in reference</i>		6					

NAME							VAPOR PRESSURE - liquid phase		
							for V/P calculation		
							liquid	liquid	
common chemical name	IUPAC #	cas # (1)	pressure	units	temp?	units	Vp	T(Vp)	data
							atm	deg K	notes
2,3,7,8-TCDD	001746-01-6		1.18E-004	Pa	25	deg C	6		
1,2,3,7,8-PeCDD	040321-76-4		4.23E-006	Pa	25	deg C	6		using value for 12347 PeCDD
1,2,3,4,7,8-HxCDD	039227-28-6		1.45E-006	Pa	25	deg C	6		
1,2,3,6,7,8-HxCDD	057653-85-7		1.45E-006	Pa	25	deg C	6		using value for 123478 HxCDD
1,2,3,7,8,9-HxCDD	019408-74-3		1.45E-006	Pa	25	deg C	6		using value for 123478 HxCDD
1,2,3,4,6,7,8-HpCDD	035822-46-9		1.77E-007	Pa	25	deg C	6		
OCDD	003268-87-9		9.53E-007	Pa	25	deg C	6		
2,3,7,8-TCDF	051207-31-9		1.99E-004	Pa	25	deg C	6		
2,3,4,7,8-PeCDF	057117-31-4		1.72E-005	Pa	25	deg C	6		
1,2,3,7,8-PeCDF	057117-41-6		1.72E-005	Pa	25	deg C	6		using value for 23478 PeCDF
1,2,3,4,7,8-HxCDF	070648-26-9		3.08E-006	Pa	25	deg C	6		
1,2,3,6,7,8-HxCDF	057117-44-9		3.61E-006	Pa	25	deg C	6		
1,2,3,7,8,9-HxCDF	072918-21-9		3.35E-006	Pa	25	deg C	6		using avg of values for 123478 HxCDF and 123678 HxCDF
2,3,4,6,7,8-HxCDF	060851-34-5		3.35E-006	Pa	25	deg C	6		using avg of values for 123478 HxCDF and 123678 HxCDF
1,2,3,4,6,7,8-HpCDF	067562-39-4		5.74E-007	Pa	25	deg C	6		
1,2,3,4,7,8,9-HpCDF	055673-89-7		5.39E-007	Pa	25	deg C	6		
OCDF	039001-02-0		1.01E-007	Pa	25	deg C	6		

VAPOR PRESSURE - liquid phase									
for V/P calculation									
liquid phase									
NAME	IUPAC #	cas # (1)	pressure	units	temp?	units	reference	Vp	T(Vp)
common chemical name								atm	deg K
biphenyl	0	000092-52-4	3.69	Pa	25	deg C	5	3.6E-005	298.15
2-PCB	1	002051-60-7	2.5	Pa	25	deg C	5	2.5E-005	298.15
3-PCB	2	002051-61-8	1	Pa	25	deg C	5	9.9E-006	298.15
4-PCB	3	002051-62-9	0.9	Pa	25	deg C	5	8.9E-006	298.15
count									
average									
standard deviation									
minimum									
maximum									
2,2'-PCB	4	013029-08-8	0.6	Pa	25	deg C	5	5.9E-006	298.15
2,3-PCB	5	016605-91-7	1.91E-004	mm Hg	25	deg C	85	2.5E-007	298.15
2,4-PCB	7	033284-50-3	0.25	Pa	25	deg C	5	2.5E-006	298.15
2,4'-PCB	8	034883-43-7	not in ref	5; see solid estim at	eft				
2,5-PCB	9	034883-39-1	0.18	Pa	25	deg C	5	1.8E-006	298.15
2,6-PCB	10	033146-45-1	not in ref	5; see solid estim at	eft				
3,3'-PCB	11	002050-67-1	0.03	Pa	25	deg C	5	3.0E-007	298.15
3,4-PCB	12	002974-92-7	not in ref	5; see solid estim at	eft				
3,5-PCB	14	034883-41-5	0.12	Pa	25	deg C	5	1.2E-006	298.15
4,4'-PCB	15	002050-68-2	0.08	Pa	25	deg C	5	7.9E-007	298.15
count									
average									
standard deviation									
minimum									
maximum									

NAME							VAPOR PRESSURE - liquid phase			
common chemical name	IUPAC #	cas # (1)	liquid	phase	vapor	at what temp	for V/P calculation		data	
							Vp atm	T(Vp) deg K		
2,2',3-PCB	16	038444-78-9			not in ref	5 or 85				
2,2',5-PCB	18	037680-65-2			0.22	Pa	25 deg C	5		
2,3,3'-PCB	20	038444-84-7			not in ref	5; see solid estim at left				
2,3,4-PCB	21	055702-46-0			not in ref	5; see solid estim at left				
2,3',5-PCB	26	038444-85-8			not in ref	5 or 85				
2,4,4'-PCB	28	007012-37-5			not in ref	5; see solid estim at left				
2,4,5-PCB	29	015862-07-4			0.044	Pa	25 deg C	5		
2,4,6-PCB	30	035693-92-6			0.09	Pa	25 deg C	5		
2,4',5,-PCB	31	016606-02-3			not in ref	5 or 85				
2',3,4-PCB	33	038444-86-9			0.003	Pa	25 deg C	5		
3,3',4-PCB	35	037680-69-6			not in ref	5 or 85				
3,4,4'-PCB	37	038444-90-5			not in ref	5 or 85				
count										
average										
standard deviation										
minimum										
maximum										
2,2',3,3'-PCB	40	038444-93-8			0.002	Pa	25 deg C	5		
2,2',3,5'-PCB	44	041464-39-5			not in ref	5; see solid estim at left				
2,2',4,4'-PCB	47	002437-79-8			0.002	Pa	25 deg C	5		
2,2',4,5'-PCB	49	041464-40-8			not in ref	5; see solid estim at left				
2,2',4,6-PCB	50	062796-65-0			not in ref	5; see solid estim at left				
2,2',4,6'-PCB	51	068194-04-7			not in ref	5 or 85				
2,2,5,5'-PCB	52	035693-99-3			0.002	Pa	25 deg C	5		
2,2,5,6'-PCB	53	041464-41-9			not in ref	5; see solid estim at left				
2,2,6,6'-PCB	54	015968-05-5			not in ref	5; see solid estim at left				
2,3,4,4'-PCB	60	033025-41-1			not in ref	5; see solid estim at left				
2,3,4,5-PCB	61	033284-53-6			not in ref	5; see solid estim at left				
2,3,5,6-PCB	65	033284-54-7			not in ref	5 or 85				
2,3,4,4'-PCB	66	032598-10-0			not in ref	5; see solid estim at left				
2,3',4',5-PCB	70	032598-11-1			not in ref	5; see solid estim at left				
2,4,4',6-PCB	75	032598-12-2			not in ref	5 or 85				
3,3',4,4'-PCB	77	032598-13-3			0.002	Pa	25 deg C	5		
3,3',5,5'-PCB	80	033284-52-5			not in ref	5; see solid estim at left				
3,4,4',5-PCB	81	070362-50-4			not in ref	5 or 85				
count										
average										
standard deviation										
minimum										
maximum										

NAME		VAPOR PRESSURE - liquid phase							
		for V/P calculation							
		liquid	phase	vapor	at what temp	Vp	T(Vp)	data	
common chemical name	IUPAC #	cas # (1)	pressure	units	temp <sup>2</sup>	units	referenc	atm	deg K
2,2',3,3',5-PCB	83	060145-20-2	not in ref	5 or 85					
2,2',3,4,5-PCB	86	065510-45-4	0.051	Pa	25	deg C	5		
2,2',3,4,5'-PCB	87	038380-02-8	0.0023	Pa	25	deg C	5		
2,2',3,4,6-PCB	88	055215-17-3	not in ref	5; see solid estim at	eft				
2,2',3,5,6-PCB	95	038379-99-6	not in ref	5 or 85					
2,2',4,4,5-PCB	99	038380-01-7	not in ref	5; see solid estim at	eft				
2,2',4,4',6-PCB	100	039485-83-1	2.22E-006	mm Hg	25	deg C	85	2.9E-009	298.15
2,2',4,5,5'-PCB	101	037680-73-2	0.0035	Pa	25	deg C	5		
2,2',4,6,6'-PCB	104	056558-16-8	not in ref	5 or 85					
2,3,3',4,4'-PCB	105	032598-14-4	not in ref	5; see solid estim at	eft				
2,3,3',4,6-PCB	110	038380-03-9	not in ref	5; see solid estim at	eft				
2,3,4,4',5-PCB	114	074472-37-0	not in ref	5 or 85					
2,3,4,5,6-PCB	116	018259-05-7	not in ref	5; see solid estim at	eft				
2,3',4,4',5-PCB	118	031508-00-6	not in ref	5 or 85					
2,3,4,5,5'-PCB	124	070424-70-3	not in ref	5 or 85					
3,3',4,4',5-PCB	126	057465-28-8	not in ref	5 or 85					
count									
average									
standard deviation									
minimum									
maximum									
2,2',3,3',4,4'-PCB	128	038380-07-3	0.00034	Pa	25	deg C	5		
2,2',3,3',4,5-PCB	129	055215-18-4	not in ref	5; see solid estim at	eft				
2,2',3,3',5,6-PCB	134	052704-70-8	not in ref	5; see solid estim at	eft				
2,2',3,3',6,6'-PCB	136	038411-22-2	not in ref	5; see solid estim at	eft				
2,2',3,4,4',5'-PCB	138	035065-28-2	not in ref	5; see solid estim at	eft				
2,2',3,4',5,6-PCB	149	038380-04-0	not in ref	5; see solid estim at	eft				
2,2',4,4',5,5'-PCB	153	035065-27-1	0.0007	Pa	25	deg C	5		
2,2',4,4',6,6'-PCB	155	033979-03-2	0.00363	Pa	25	deg C	5		
2,3,3',4,4',5-PCB	156	038380-08-4	not in ref	5; see solid estim at	eft				
2,3,3',4,4',5'-PCB	157	069782-90-7	not in ref	5 or 85					
2,3',4,4',5,5'-PCB	167	052663-72-6	not in ref	5; see solid estim at	eft				
3,3',4,4',5,5'-PCB	169	032774-16-6	not in ref	5; see solid estim at	eft				
count									
average									
standard deviation									
minimum									
maximum									

VAPOR PRESSURE - liquid phase							
for V/P calculation							
NAME		liquid	phase	vapor	at what temp	Vp	T(Vp)
common chemical name	IUPAC #	cas # (1)	pressure	units	temp <sup>2</sup> units	reference	atm deg K
2,2',3,3',4,4',5-PCB	170	035065-30-6	not in ref	5; see solid estim at left			
2,2',3,3',4,4',6-PCB	171	052663-71-5	0.00025	Pa	25 deg C	5	
2,2',3,4,4',5,5'-PCB	180	035065-29-3	not in ref	5; see solid estim at left			
2,2',3,4,5,5',6-PCB	185	052712-05-7	not in ref	5; see solid estim at left			
2,2',3,4',5,5',6-PCB	187	052663-68-0	not in ref	5; see solid estim at left			
2,3,3',4,4',5,5'-PCB	189	039635-31-9	not in ref 5 or 85				
count							
average							
standard deviation							
minimum							
maximum							
2,2',3,3',4,4',5,5'-PCB	194	035694-08-7	not in ref	5; see solid estim at left			
2,2',3,3',5,5',6,6'-PCB	202	002136-99-4	0.0006	Pa	25 deg C	5	
count							
average							
standard deviation							
minimum							
maximum							
2,2',3,3',4,4',5,5',6-PCB	206	040186-72-9	1.2E-005	Pa	25 deg C	5	
2,2',3,3',4,4',5,6,6'-PCB	207	052663-79-3	not in ref 5 or 85				
2,2',3,3',4,5,5',6,6'-PCB	208	052663-77-1	not in ref	5; see solid estim at left			
count							
average							
standard deviation							
minimum							
maximum							
2,2',3,3',4,4',5,5',6,6'-PCB	209	002051-24-3	0.00003	Pa	25 deg C	5	

WATER SOLUBILITY- 1						
relative to most stable condensed phase						
		water	at what	temp	data	
common chemical name	IUPAC #	cas # (1)	solubility	units	temp?	units
octachlorostyrene		029082-74-4				
4-bromophenyl phenyl ether		000101-55-3	4.8 g/m3	25	deg C	7
3,3'-dichlorobenzidine		000091-94-1	3.1 mg/lit	25	deg C	Banerjee et al same in ref 8
1,3-dinitropyrene		075321-20-9	0.0132 g/m3	25	deg C	crude estim =pyrene / 10
1,6-dinitropyrene		042397-64-8	0.0132 g/m3	25	deg C	crude estim =pyrene / 10
1,8-dinitropyrene		042397-65-9	0.0132 g/m3	25	deg C	crude estim =pyrene / 10
2,7-dinitropyrene		117929-15-4	0.0132 g/m3	25	deg C	crude estim =pyrene / 10
dinitropyrenes (mixed)		078432-19-6				
hexachloro-1,3-butadiene		000087-68-3	3.2 g/m3	25	deg C	7
4,4'-methylene bis(2-chloroaniline)		000101-14-4	13.9 mg/liter	24	deg C	17
pentachlorophenol		000087-86-5	14 g/m3	25	deg C	8
aldrin		000309-00-2	0.02 mg/liter	20	deg C	49
dieldrin		000060-57-1	0.17 mg/liter	20	deg C	49
p,p'-DDT		000050-29-3	5.4 ug/liter	24	deg C	63 a lot of conflicting data
p,p'-DDD		000072-54-8	90 ppb	25	deg C	64 other data as well
p,p'-DDE		000072-55-9	120 ppb	25	deg C	64 other data as well
heptachlor		000076-44-8	0.18 mg/lit	temp not stated		26
heptachlor epoxide		001024-57-3	0.2 mg/lit	temp not stated		26
methoxychlor		000072-43-5	0.045 mg/lit	25	deg C	26
mirex		002385-85-5	0.6 mg/lit	temp not stated		67 other data presented
toxaphene		008001-35-2				
endrin		000072-20-8	0.25 ug/liter	25	deg C	26
alpha-hexachlorocyclohexane		000319-84-6	10 ppm	temp not reported		34
beta-hexachlorocyclohexane		000319-85-7	5 ppm	temp not reported		34
delta-hexachlorocyclohexane		000319-86-8	10 ppm	temp not reported		34
gamma-hexachlorocyclohexane		000058-89-9	17 ppm	temp not reported		35
mixed hexachlorocyclohexanes		000319-84-6				

WATER SOLUBILITY- 1						
relative to most stable condensed phase						
		water	at what	temp	reference	data
common chemical name	IUPAC #	cas # (1)	solubility	units	temp?	units
cadmium	007440-43-9		"insoluble"			76
cadmium carbonate	000513-78-0		"practically insoluble"			74
cadmium chloride	010108-64-2		1400 g/liter	20	deg C	72 other data at other temps
cadmium oxide	001306-19-0		5 mg/liter	temp not stated		74
cadmium sulfate	010124-36-4		750 g/liter	0 deg C		72 other data at other temps
cadmium sulfide	001306-23-6		1.3 mg/lit	18 deg C		74
elemental mercury	007439-97-6		0.00000006 g/mL	25	deg C	95
mercury oxide	021908-53-2					ref 95: no data
mercuric chloride	007487-94-7		7.4E+004 mg/lit	25	deg C	95
monomethyl mercury chloride	000115-09-3					ref 95: no data
dimethyl mercury	000593-74-8					ref 95: no data
tetraethyl lead	000078-00-2		0.21 mg/lit	26	deg C	85
tetramethyl lead	000075-74-1		9 mg/lit	not stated		97 citing 98 estm?
triethyl lead radical (1+ cation)	014570-15-1					
triethyl lead hydride	005224-23-7					
triethyl lead chloride	001067-14-7					
diethyl lead radical (2+ cation)	024952-65-6					
diethyl lead dihydride	081494-11-3					
diethyl lead dichloride	013231-90-8					
trimethyl lead radical (1+ cation)	014570-16-2					
trimethyl lead hydride	007442-13-9					
trimethyl lead chloride	001520-78-1					
dimethyl lead radical (2+ cation)	021774-13-0					
dimethyl lead dihydride	030691-92-0					
dimethyl lead dichloride	001520-77-0					
bis (tributyltin) oxide	000056-35-9		4 mg/lit	20	deg C	97 expt'l
tributyl tin	000688-75-3					
tributyltin fluoride	001983-10-4					
tributyltin chloride	001461-22-9					
tributyltin hydroxide	001067-97-6					
tributyltin naphthenate						
tris(tributylstanny) phosphate	013435-05-7					

WATER SOLUBILITY- 1						
relative to most stable condensed phase						
NAME		water	at what	temp	reference	data
common chemical name	IUPAC #	cas # (1)	solubility	units	temp?	units
1,4-dichlorobenzene	000106-46-7		83	g/m3	25	deg C
1,2,3,4-tetrachlorobenzene	000634-66-2		7.8	g/m3	25	deg C
1,2,4,5-tetrachlorobenzene	000095-94-3		1.27	g/m3	25	deg C
1,2,3,5-tetrachlorobenzene	000634-90-2		3.6	g/m3	25	deg C
pentachlorobenzene	000608-93-5		0.65	g/m3	25	deg C
hexachlorobenzene	000118-74-1		0.005	g/m3	25	deg C
naphthalene	000091-20-3		31	g/m3	25	deg C
acenaphthene	000083-32-9		3.8	g/m3	25	deg C
acenaphthylene	000208-96-8		16.1	g/m3	25	deg C
fluorene	000086-73-7		1.9	g/m3	25	deg C
phenanthrene	000085-01-8		1.1	g/m3	25	deg C
anthracene	000120-12-7		0.045	g/m3	25	deg C
pyrene	000129-00-0		0.132	g/m3	25	deg C
fluoranthene	000206-44-0		0.26	g/m3	25	deg C
chrysene	000218-01-9		2.8E-003	mg/lit	temp not reported	14
benz [ a ] anthracene	000056-55-3		0.011	g/m3	25	deg C
benzo [ b ] fluoranthene	000205-99-2		0.0015	g/m3	25	deg C
benzo [ j ] fluoranthene	000205-82-3		0.0025	g/m3	25	deg C
benzo [ k ] fluoranthene	000207-08-9		0.0008	g/m3	25	deg C
benzo [ a ] pyrene	000050-32-8		0.0038	g/m3	25	deg C
benzo [ e ] pyrene	000192-97-2		0.004	g/m3	25	deg C
perylene	000198-55-0		0.0004	g/m3	25	deg C
benzo [ g,h,i ] perylene	000191-24-2		0.00026	g/m3	25	deg C
dibenz [ a,h ] anthracene	000053-70-3		0.0006	g/m3	25	deg C
indeno [ 1,2,3-c,d ] pyrene	000193-39-5		0.062	mg/lit	temp not reported	9

WATER SOLUBILITY- 1						
relative to most stable condensed phase						
NAME		water	at what	temp	reference	data
common chemical name	IUPAC #	cas # (1)	solubility	units	temp?	units
2,3,7,8-TCDD	001746-01-6		0.0193	mg/m3	25	deg C
1,2,3,7,8-PeCDD	040321-76-4		0.118	mg/m3	25	deg C
1,2,3,4,7,8-HxCDD	039227-28-6		0.00442	mg/m3	25	deg C
1,2,3,6,7,8-HxCDD	057653-85-7		0.00442	mg/m3	25	deg C
1,2,3,7,8,9-HxCDD	019408-74-3		0.00442	mg/m3	25	deg C
1,2,3,4,6,7,8-HpCDD	035822-46-9		0.0024	mg/m3	25	deg C
OCDD	003268-87-9		0.000074	mg/m3	25	deg C
2,3,7,8-TCDF	051207-31-9		0.419	mg/m3	25	deg C
2,3,4,7,8-PeCDF	057117-31-4		0.236	mg/m3	25	deg C
1,2,3,7,8-PeCDF	057117-41-6		0.236	mg/m3	25	deg C
1,2,3,4,7,8-HxCDF	070648-26-9		0.00825	mg/m3	25	deg C
1,2,3,6,7,8-HxCDF	057117-44-9		0.0177	mg/m3	25	deg C
1,2,3,7,8,9-HxCDF	072918-21-9		0.012975	mg/m3	25	deg C
2,3,4,6,7,8-HxCDF	060851-34-5		0.012975	mg/m3	25	deg C
1,2,3,4,6,7,8-HpCDF	067562-39-4		0.00135	mg/m3	25	deg C
1,2,3,4,7,8,9-HpCDF	055673-89-7		0.00135	mg/m3	25	deg C
OCDF	039001-02-0		0.00116	mg/m3	25	deg C

WATER SOLUBILITY- 1						
relative to most stable condensed phase						
			water	at what	temp	data
common chemical name	IUPAC #	cas # (1)	solubility	units	temp?	units
biphenyl	0	000092-52-4	7	g/m3	25	deg C
2-PCB	1	002051-60-7	5.5	g/m3	25	deg C
3-PCB	2	002051-61-8	2.5	g/m3	25	deg C
4-PCB	3	002051-62-9	1.2	g/m3	25	deg C
count						
average						
standard deviation						
minimum						
maximum						
2,2'-PCB	4	013029-08-8	1	g/m3	25	deg C
2,3-PCB	5	016605-91-7	not in reference 5			
2,4-PCB	7	033284-50-3	1.25	g/m3	25	deg C
2,4'-PCB	8	034883-43-7	1	g/m3	25	deg C
2,5-PCB	9	034883-39-1	2	g/m3	25	deg C
2,6-PCB	10	033146-45-1	1.4	g/m3	25	deg C
3,3'-PCB	11	002050-67-1	0.354	g/m3	25	deg C
3,4-PCB	12	002974-92-7	0.008	g/m3	25	deg C
3,5-PCB	14	034883-41-5	not in reference 5			
4,4'-PCB	15	002050-68-2	0.06	g/m3	25	deg C
count						
average						
standard deviation						
minimum						
maximum						

WATER SOLUBILITY- 1							
relative to most stable condensed phase							
NAME			water	at what	temp	data	
common chemical name	IUPAC #	cas # (1)	solubility	units	temp?	units	reference notes
2,2',3-PCB	16	038444-78-9			-----not in reference 5-----		
2,2',5-PCB	18	037680-65-2	0.4	g/m3	25	deg C	5
2,3,3'-PCB	20	038444-84-7			-----not in reference 5-----		
2,3,4-PCB	21	055702-46-0			-----not in reference 5-----		
2,3',5-PCB	26	038444-85-8	0.251	g/m3	25	deg C	5
2,4,4'-PCB	28	007012-37-5	0.16	g/m3	25	deg C	5
2,4,5-PCB	29	015862-07-4	0.14	g/m3	25	deg C	5
2,4,6-PCB	30	035693-92-6	0.2	g/m3	25	deg C	5
2,4',5,-PCB	31	016606-02-3			-----not in reference 5-----		
2',3,4-PCB	33	038444-86-9	0.08	g/m3	25	deg C	5
3,3',4-PCB	35	037680-69-6			-----not in reference 5-----		
3,4,4'-PCB	37	038444-90-5	0.015	g/m3	25	deg C	5
count							
average							
standard deviation							
minimum							
maximum							
2,2',3,3'-PCB	40	038444-93-8	0.03	g/m3	25	deg C	5
2,2',3,5'-PCB	44	041464-39-5	0.1	g/m3	25	deg C	5
2,2',4,4'-PCB	47	002437-79-8	0.09	g/m3	25	deg C	5
2,2',4,5'-PCB	49	041464-40-8	0.016	g/m3	25	deg C	5
2,2',4,6-PCB	50	062796-65-0			-----not in reference 5-----		
2,2',4,6'-PCB	51	068194-04-7			-----not in reference 5-----		
2,2,5,5'-PCB	52	035693-99-3	0.03	g/m3	25	deg C	5
2,2,5,6'-PCB	53	041464-41-9			-----not in reference 5-----		
2,2,6,6'-PCB	54	015968-05-5			-----not in reference 5-----		
2,3,4,4'-PCB	60	033025-41-1			-----not in reference 5-----		
2,3,4,5-PCB	61	033284-53-6	0.02	g/m3	25	deg C	5
2,3,5,6-PCB	65	033284-54-7			-----not in reference 5-----		
2,3,4,4'-PCB	66	032598-10-0	0.04	g/m3	25	deg C	5
2,3',4',5-PCB	70	032598-11-1			-----not in reference 5-----		
2,4,4',6-PCB	75	032598-12-2	0.091	g/m3	25	deg C	5
3,3',4,4'-PCB	77	032598-13-3	0.001	g/m3	25	deg C	5
3,3',5,5'-PCB	80	033284-52-5	0.0012	g/m3	25	deg C	5
3,4,4',5-PCB	81	070362-50-4			-----not in reference 5-----		
count							
average							
standard deviation							
minimum							
maximum							

WATER SOLUBILITY- 1							
relative to most stable condensed phase							
NAME			water	at what	temp	reference	data
common chemical name	IUPAC #	cas # (1)	solubility	units	temp?	units	notes
2,2',3,3',5-PCB	83	060145-20-2		-----	not in reference 5		
2,2',3,4,5-PCB	86	065510-45-4	0.02	g/m3	25	deg C	5
2,2',3,4,5'-PCB	87	038380-02-8	0.004	g/m3	25	deg C	5
2,2',3,4,6-PCB	88	055215-17-3	0.012	g/m3	25	deg C	5
2,2',3,5,6-PCB	95	038379-99-6		-----	not in reference 5		
2,2',4,4',5-PCB	99	038380-01-7		-----	not in reference 5		
2,2',4,4',6-PCB	100	039485-83-1		-----	not in reference 5		
2,2',4,5,5'-PCB	101	037680-73-2	0.01	g/m3	25	deg C	5
2,2',4,6,6'-PCB	104	056658-16-8	0.0156	g/m3	25	deg C	5
2,3,3',4,4'-PCB	105	032598-14-4		-----	not in reference 5		
2,3,3',4,6-PCB	110	038380-03-9	0.004	g/m3	25	deg C	5
2,3,4,4',5-PCB	114	074472-37-0		-----	not in reference 5		
2,3,4,5,6-PCB	116	018259-05-7	0.008	g/m3	25	deg C	5
2,3',4,4',5-PCB	118	031508-00-6		-----	not in reference 5		
2,3,4,5,5'-PCB	124	070424-70-3		-----	not in reference 5		
3,3',4,4',5-PCB	126	057465-28-8		-----	not in reference 5		
count							
average							
standard deviation							
minimum							
maximum							
2,2',3,3',4,4'-PCB	128	038380-07-3	0.0006	g/m3	25	deg C	5
2,2',3,3',4,5-PCB	129	055215-18-4	0.0006	g/m3	25	deg C	5
2,2',3,3',5,6-PCB	134	052704-70-8	0.0004	g/m3	25	deg C	5
2,2',3,3',6,6'-PCB	136	038411-22-2	0.0008	g/m3	25	deg C	5
2,2',3,4,4',5-PCB	138	035065-28-2		-----	not in reference 5		
2,2',3,4,5,6-PCB	149	038380-04-0		-----	not in reference 5		
2,2',4,4',5,5'-PCB	153	035065-27-1	0.001	g/m3	25	deg C	5
2,2',4,4',6,6'-PCB	155	033979-03-2	0.002	g/m3	25	deg C	5
2,3,3',4,4',5-PCB	156	038380-08-4		-----	not in reference 5		
2,3,3',4,4',5'-PCB	157	069782-90-7		-----	not in reference 5		
2,3',4,4',5,5'-PCB	167	052663-72-6		-----	not in reference 5		
3,3',4,4',5,5'-PCB	169	032774-16-6		-----	not in reference 5		
count							
average							
standard deviation							
minimum							
maximum							

WATER SOLUBILITY- 1						
relative to most stable condensed phase						
		water	at what	temp	reference	data
common chemical name	IUPAC #	cas # (1)	solubility	units	temp?	units
2,2',3,3',4,4',5-PCB	170	035065-30-6	-----	not in reference 5	-----	-----
2,2',3,3',4,4',6-PCB	171	052663-71-5	0.002	g/m3	25 deg C	5
2,2',3,4,4',5,5'-PCB	180	035065-29-3	-----	not in reference 5	-----	-----
2,2',3,4,5,5',6-PCB	185	052712-05-7	0.00045	g/m3	25 deg C	5
2,2',3,4',5,5',6-PCB	187	052663-68-0	-----	not in reference 5	-----	-----
2,3,3',4,4',5,5'-PCB	189	039635-31-9	-----	not in reference 5	-----	-----
count						
average						
standard deviation						
minimum						
maximum						
2,2',3,3',4,4',5,5'-PCB	194	035694-08-7	0.0002	g/m3	25 deg C	5
2,2',3,3',5,5',6,6'-PCB	202	002136-99-4	0.0003	g/m3	25 deg C	5
count						
average						
standard deviation						
minimum						
maximum						
2,2',3,3',4,4',5,5',6-PCB	206	040186-72-9	0.00011	g/m3	25 deg C	5
2,2',3,3',4,4',5,6,6'-PCB	207	052663-79-3	-----	not in reference 5	-----	-----
2,2',3,3',4,5,5',6,6'-PCB	208	052663-77-1	0.000018	g/m3	25 deg C	5
count						
average						
standard deviation						
minimum						
maximum						
2,2',3,3',4,4',5,5',6,6'-PCB	209	002051-24-3	0.000001	g/m3	25 deg C	5

WATER SOLUBILITY- 2						
relative to most stable condensed phase						
		water	at what	temp		data
common chemical name	IUPAC #	cas # (1)	solubility	units	temp?	units
octachlorostyrene		029082-74-4				
4-bromophenyl phenyl ether		000101-55-3	0.0193	mol/m3	25	deg C
3,3'-dichlorobenzidine		000091-94-1	0.0122	mol/m3	25	deg C
1,3-dinitropyrene		075321-20-9	0.132	g/m3	25	deg C
1,6-dinitropyrene		042397-64-8	0.132	g/m3	25	deg C
1,8-dinitropyrene		042397-65-9	0.132	g/m3	25	deg C
2,7-dinitropyrene		117929-15-4	0.132	g/m3	25	deg C
dinitropyrenes (mixed)		078432-19-6				
hexachloro-1,3-butadiene		000087-68-3	0.013	mol/m3	25	deg C
4,4'-methylene bis(2-chloroaniline)		000101-14-4				
pentachlorophenol		000087-86-5	0.053	mol/m3	25	deg C
aldrin		000309-00-2				
die�din		000060-57-1				
p,p'-DDT		000050-29-3				
p,p'-DDD		000072-54-8				
p,p'-DDE		000072-55-9				
heptachlor		000076-44-8				
heptachlor epoxide		001024-57-3				
methoxychlor		000072-43-5				
mirex		002385-85-5				
toxaphene		008001-35-2				
endrin		000072-20-8				
alpha-hexachlorocyclohexane		000319-84-6				
beta-hexachlorocyclohexane		000319-85-7				
delta-hexachlorocyclohexane		000319-86-8				
gamma-hexachlorocyclohexane		000058-89-9				
mixed hexachlorocyclohexanes		000319-84-6				

WATER SOLUBILITY- 2							
relative to most stable condensed phase							
NAME		water	at what	temp		data	
common chemical name	IUPAC #	cas # (1)	solubility	units	temp?	units	reference notes
cadmium		007440-43-9					
cadmium carbonate		000513-78-0					
cadmium chloride		010108-64-2					
cadmium oxide		001306-19-0					
cadmium sulfate		010124-36-4					
cadmium sulfide		001306-23-6					
elemental mercury		007439-97-6					
mercury oxide		021908-53-2					
mercuric chloride		007487-94-7					
monomethyl mercury chloride		000115-09-3					
dimethyl mercury		000593-74-8					
tetraethyl lead		000078-00-2					
tetramethyl lead		000075-74-1					
triethyl lead radical (1+ cation)		014570-15-1					
triethyl lead hydride		005224-23-7					
triethyl lead chloride		001067-14-7					
diethyl lead radical (2+ cation)		024952-65-6					
diethyl lead dihydride		081494-11-3					
diethyl lead dichloride		013231-90-8					
trimethyl lead radical (1+ cation)		014570-16-2					
trimethyl lead hydride		007442-13-9					
trimethyl lead chloride		001520-78-1					
dimethyl lead radical (2+ cation)		021774-13-0					
dimethyl lead dihydride		030691-92-0					
dimethyl lead dichloride		001520-77-0					
bis (tributyltin) oxide		000056-35-9					
tributyl tin		000688-75-3					
tributyltin fluoride		001983-10-4					
tributyltin chloride		001461-22-9					
tributyltin hydroxide		001067-97-6					
tributyltin naphthenate							
tris(tributylstanny) phosphate		013435-05-7					

WATER SOLUBILITY- 2							
relative to most stable condensed phase							
		water	at what	temp	reference	data	
common chemical name	IUPAC #	cas # (1)	solubility	units	temp?	units	
1,4-dichlorobenzene	000106-46-7		0.5646	mol/m3	25	deg C	5
1,2,3,4-tetrachlorobenzene	000634-66-2		0.0361	mol/m3	25	deg C	5
1,2,4,5-tetrachlorobenzene	000095-94-3		0.00588	mol/m3	25	deg C	5
1,2,3,5-tetrachlorobenzene	000634-90-2		0.0167	mol/m3	25	deg C	5
pentachlorobenzene	000608-93-5		0.0026	mol/m3	25	deg C	5
hexachlorobenzene	000118-74-1		0.0000176	mol/m3	25	deg C	5
naphthalene	000091-20-3		241.83	mmol/m3	25	deg C	6
acenaphthene	000083-32-9		24.642	mmol/m3	25	deg C	6
acenaphthylene	000208-96-8		107.19	mmol/m3	25	deg C	6
fluorene	000086-73-7		11.43	mmol/m3	25	deg C	6
phenanthrene	000085-01-8		6.173	mmol/m3	25	deg C	6
anthracene	000120-12-7		0.253	mmol/m3	25	deg C	6
pyrene	000129-00-0		0.652	mmol/m3	25	deg C	6
fluoranthene	000206-44-0		1.186	mmol/m3	25	deg C	6
chrysene	000218-01-9		not given in reference 6				
benz [ a ] anthracene	000056-55-3		0.0482	mmol/m3	25	deg C	6
benzo [ b ] fluoranthene	000205-99-2		0.00595	mmol/m3	25	deg C	6
benzo [ j ] fluoranthene	000205-82-3		0.0099	mmol/m3	25	deg C	6
benzo [ k ] fluoranthene	000207-08-9		0.00317	mmol/m3	25	deg C	6
benzo [ a ] pyrene	000050-32-8		0.0151	mmol/m3	25	deg C	6
benzo [ e ] pyrene	000192-97-2		0.0159	mmol/m3	25	deg C	6
perylene	000198-55-0		0.00159	mmol/m3	25	deg C	6
benzo [ g,h,i ] perylene	000191-24-2		0.000968	mmol/m3	25	deg C	6
dibenz [ a,h ] anthracene	000053-70-3		0.00216	mmol/m3	25	deg C	6
indeno [ 1,2,3-c,d ] pyrene	000193-39-5		not given in reference 6				

WATER SOLUBILITY- 2						
relative to most stable condensed phase						
NAME		water	at what	temp	reference	data
common chemical name	IUPAC #	cas # (1)	solubility	units	temp?	units
2,3,7,8-TCDD		001746-01-6	6.00E-005	mmol/m3	25 deg C	6
1,2,3,7,8-PeCDD		040321-76-4	3.31E-004	mmol/m3	25 deg C	6 using value for 12347 PeCDD
1,2,3,4,7,8-HxCDD		039227-28-6	1.13E-005	mmol/m3	25 deg C	6
1,2,3,6,7,8-HxCDD		057653-85-7	1.13E-005	mmol/m3	25 deg C	6 using value for 123478 HxCDD
1,2,3,7,8,9-HxCDD		019408-74-3	1.13E-005	mmol/m3	25 deg C	6 using value for 123478 HxCDD
1,2,3,4,6,7,8-HpCDD		035822-46-9	5.64E-006	mmol/m3	25 deg C	6
OCDD		003268-87-9	1.61E-007	mmol/m3	25 deg C	6
2,3,7,8-TCDF		051207-31-9	1.37E-003	mmol/m3	25 deg C	6
2,3,4,7,8-PeCDF		057117-31-4	6.93E-004	mmol/m3	25 deg C	6
1,2,3,7,8-PeCDF		057117-41-6	6.93E-004	mmol/m3	25 deg C	6 using value for 23478 PeCDF
1,2,3,4,7,8-HxCDF		070648-26-9	2.20E-005	mmol/m3	25 deg C	6
1,2,3,6,7,8-HxCDF		057117-44-9	4.72E-005	mmol/m3	25 deg C	6
1,2,3,7,8,9-HxCDF		072918-21-9	3.46E-005	mmol/m3	25 deg C	6 using avg of values for 123478 HxCDF and 123678 HxCDF
2,3,4,6,7,8-HxCDF		060851-34-5	3.46E-005	mmol/m3	25 deg C	6 using avg of values for 123478 HxCDF and 123678 HxCDF
1,2,3,4,6,7,8-HpCDF		067562-39-4	3.3E-006	mmol/m3	25 deg C	6
1,2,3,4,7,8,9-HpCDF		055673-89-7	3.3E-006	mmol/m3	25 deg C	6 using value for 1234678 HpCDF
OCDF		039001-02-0	2.61E-006	mmol/m3	25 deg C	6

WATER SOLUBILITY- 2						
relative to most stable condensed phase						
		water	at what	temp	reference	data
common chemical name	IUPAC #	cas # (1)	solubility	units	temp?	units
biphenyl	0	000092-52-4	45.39	mmol/m3	25	deg C
2-PCB	1	002051-60-7	29.15	mmol/m3	25	deg C
3-PCB	2	002051-61-8	13.25	mmol/m3	25	deg C
4-PCB	3	002051-62-9	6.36	mmol/m3	25	deg C
count						
average						
standard deviation						
minimum						
maximum						
2,2'-PCB	4	013029-08-8	4.48	mmol/m3	25	deg C
2,3-PCB	5	016605-91-7	<i>not in reference 5</i>			
2,4-PCB	7	033284-50-3	5.6	mmol/m3	25	deg C
2,4'-PCB	8	034883-43-7	4.48	mmol/m3	25	deg C
2,5-PCB	9	034883-39-1	8.96	mmol/m3	25	deg C
2,6-PCB	10	033146-45-1	6.28	mmol/m3	25	deg C
3,3'-PCB	11	002050-67-1	1.587	mmol/m3	25	deg C
3,4-PCB	12	002974-92-7	<i>not in reference 5</i>			
3,5-PCB	14	034883-41-5	<i>not in reference 5</i>			
4,4'-PCB	15	002050-68-2	0.269	mmol/m3	25	deg C
count						
average						
standard deviation						
minimum						
maximum						

WATER SOLUBILITY- 2							
relative to most stable condensed phase							
NAME			water	at what	temp	reference	data
common chemical name	IUPAC #	cas # (1)	solubility	units	temp?	units	notes
2,2',3-PCB	16	038444-78-9	-----	not in reference 5 -----			
2,2',5-PCB	18	037680-65-2	1.55	mmol/m3	25	deg C	5
2,3,3'-PCB	20	038444-84-7	-----	not in reference 5 -----			
2,3,4-PCB	21	055702-46-0	-----	not in reference 5 -----			
2,3',5-PCB	26	038444-85-8	0.975	mmol/m3	25	deg C	5
2,4,4'-PCB	28	007012-37-5	0.621	mmol/m3	25	deg C	5
2,4,5-PCB	29	015862-07-4	0.544	mmol/m3	25	deg C	5
2,4,6-PCB	30	035693-92-6	0.777	mmol/m3	25	deg C	5
2,4',5,-PCB	31	016606-02-3	-----	not in reference 5 -----			
2',3,4-PCB	33	038444-86-9	0.311	mmol/m3	25	deg C	5
3,3',4-PCB	35	037680-69-6	-----	not in reference 5 -----			
3,4,4'-PCB	37	038444-90-5	0.0582	mmol/m3	25	deg C	5
count							
average							
standard deviation							
minimum							
maximum							
2,2',3,3'-PCB	40	038444-93-8	0.103	mmol/m3	25	deg C	5
2,2',3,5'-PCB	44	041464-39-5	0.342	mmol/m3	25	deg C	5
2,2',4,4'-PCB	47	002437-79-8	0.308	mmol/m3	25	deg C	5
2,2',4,5'-PCB	49	041464-40-8	0.0548	mmol/m3	25	deg C	5
2,2',4,6-PCB	50	062796-65-0	-----	not in reference 5 -----			
2,2',4,6'-PCB	51	068194-04-7	-----	not in reference 5 -----			
2,2,5,5'-PCB	52	035693-99-3	0.103	mmol/m3	25	deg C	5
2,2,5,6'-PCB	53	041464-41-9	-----	not in reference 5 -----			
2,2,6,6'-PCB	54	015968-05-5	-----	not in reference 5 -----			
2,3,4,4'-PCB	60	033025-41-1	-----	not in reference 5 -----			
2,3,4,5-PCB	61	033284-53-6	0.0685	mmol/m3	25	deg C	5
2,3,5,6-PCB	65	033284-54-7	-----	not in reference 5 -----			
2,3,4,4'-PCB	66	032598-10-0	0.0147	mmol/m3	25	deg C	5
2,3',4',5-PCB	70	032598-11-1	-----	not in reference 5 -----			
2,4,4',6-PCB	75	032598-12-2	-----	not in reference 5 -----			
3,3',4,4'-PCB	77	032598-13-3	0.0342	mmol/m3	25	deg C	5
3,3',5,5'-PCB	80	033284-52-5	0.0041	mmol/m3	25	deg C	5
3,4,4',5-PCB	81	070362-50-4	-----	not in reference 5 -----			
count							
average							
standard deviation							
minimum							
maximum							

WATER SOLUBILITY- 2							
relative to most stable condensed phase							
			water	at what	temp	reference	data
common chemical name	IUPAC #	cas # (1)	solubility	units	temp?	units	notes
2,2',3,3',5-PCB	83	060145-20-2		-----	not in reference 5		
2,2',3,4,5-PCB	86	065510-45-4	0.0613	mmol/m3	25	deg C	5
2,2',3,4,5'-PCB	87	038380-02-8	0.0123	mmol/m3	25	deg C	5
2,2',3,4,6-PCB	88	055215-17-3	0.0368	mmol/m3	25	deg C	5
2,2',3,5,6-PCB	95	038379-99-6		-----	not in reference 5		
2,2',4,4,5-PCB	99	038380-01-7		-----	not in reference 5		
2,2',4,4,6-PCB	100	039485-83-1		-----	not in reference 5		
2,2',4,5,5'-PCB	101	037680-73-2	0.0306	mmol/m3	25	deg C	5
2,2',4,6,6'-PCB	104	056558-16-8	0.0306	mmol/m3	25	deg C	5
2,3,3',4,4'-PCB	105	032598-14-4		-----	not in reference 5		
2,3,3',4,6-PCB	110	038380-03-9		-----	not in reference 5		
2,3,4,4',5-PCB	114	074472-37-0		-----	not in reference 5		
2,3,4,5,6-PCB	116	018259-05-7	0.0145	mmol/m3	25	deg C	5
2,3',4,4',5-PCB	118	031508-00-6		-----	not in reference 5		
2,3,4,5,5'-PCB	124	070424-70-3		-----	not in reference 5		
3,3',4,4',5-PCB	126	057465-28-8		-----	not in reference 5		
count							
average							
standard deviation							
minimum							
maximum							
2,2',3,3',4,4'-PCB	128	038380-07-3	0.00166	mmol/m3	25	deg C	5
2,2',3,3',4,5-PCB	129	055215-18-4	0.00166	mmol/m3	25	deg C	5
2,2',3,3',5,6-PCB	134	052704-70-8	0.00111	mmol/m3	25	deg C	5
2,2',3,3',6,6'-PCB	136	038411-22-2	0.00222	mmol/m3	25	deg C	5
2,2',3,4,4',5'-PCB	138	035065-28-2		-----	not in reference 5		
2,2',3,4,5',6-PCB	149	038380-04-0		-----	not in reference 5		
2,2',4,4',5,5'-PCB	153	035065-27-1	0.00277	mmol/m3	25	deg C	5
2,2',4,4',6,6'-PCB	155	033979-03-2	0.0055	mmol/m3	25	deg C	5
2,3,3',4,4',5-PCB	156	038380-08-4		-----	not in reference 5		
2,3,3',4,4',5'-PCB	157	069782-90-7		-----	not in reference 5		
2,3',4,4',5,5'-PCB	167	052663-72-6		-----	not in reference 5		
3,3',4,4',5,5'-PCB	169	032774-16-6		-----	not in reference 5		
count							
average							
standard deviation							
minimum							
maximum							

WATER SOLUBILITY- 2						
relative to most stable condensed phase						
		water	at what	temp	reference	data
common chemical name	IUPAC #	cas # (1)	solubility	units	temp?	units
2,2',3,3',4,4',5-PCB	170	035065-30-6	-----	not in reference 5	-----	-----
2,2',3,3',4,4',6-PCB	171	052663-71-5	0.00506	mmol/m3	25 deg C	5
2,2',3,4,4',5,5'-PCB	180	035065-29-3	-----	not in reference 5	-----	-----
2,2',3,4,5,5',6-PCB	185	052712-05-7	0.00114	mmol/m3	25 deg C	5
2,2',3,4',5,5',6-PCB	187	052663-68-0	-----	not in reference 5	-----	-----
2,3,3',4,4',5,5'-PCB	189	039635-31-9	-----	not in reference 5	-----	-----
count						
average						
standard deviation						
minimum						
maximum						
2,2',3,3',4,4',5,5'-PCB	194	035694-08-7	0.00047	mmol/m3	25 deg C	5
2,2',3,3',5,5',6,6'-PCB	202	002136-99-4	0.0007	mmol/m3	25 deg C	5
count						
average						
standard deviation						
minimum						
maximum						
2,2',3,3',4,4',5,5',6-PCB	206	040186-72-9	0.000237	mmol/m3	25 deg C	5
2,2',3,3',4,4',5,6,6'-PCB	207	052663-79-3	-----	not in reference 5	-----	-----
2,2',3,3',4,5,5',6,6'-PCB	208	052663-77-1	0.000038	mmol/m3	25 deg C	5
count						
average						
standard deviation						
minimum						
maximum						
2,2',3,3',4,4',5,5',6,6'-PCB	209	002051-24-3	0.000002	mmol/m3	25 deg C	5

WATER SOLUBILITY- 3						
relative to subcooled liquid						
NAME		water	at what	temp	reference	data
common chemical name	IUPAC #	cas # (1)	solubility	units	temp?	units
octachlorostyrene		029082-74-4				
4-bromophenyl phenyl ether		000101-55-3	0.0193	mol/m3	25	deg C
3,3'-dichlorobenzidine		000091-94-1	0.14	mol/m3	25	deg C
1,3-dinitropyrene		075321-20-9				
1,6-dinitropyrene		042397-64-8				
1,8-dinitropyrene		042397-65-9				
2,7-dinitropyrene		117929-15-4				
dinitropyrenes (mixed)		078432-19-6				
hexachloro-1,3-butadiene		000087-68-3	0.013	mol/m3	25	deg C
4,4'-methylene bis(2-chloroaniline)		000101-14-4				
pentachlorophenol		000087-86-5	1.565	mol/m3	25	deg C
aldrin		000309-00-2				
dieleldrin		000060-57-1				
p,p'-DDT		000050-29-3				
p,p'-DDD		000072-54-8				
p,p'-DDE		000072-55-9				
heptachlor		000076-44-8				
heptachlor epoxide		001024-57-3				
methoxychlor		000072-43-5				
mirex		002385-85-5				
toxaphene		008001-35-2	0.55	mg/lit	20	deg C
endrin		000072-20-8				
alpha-hexachlorocyclohexane		000319-84-6				
beta-hexachlorocyclohexane		000319-85-7				
delta-hexachlorocyclohexane		000319-86-8				
gamma-hexachlorocyclohexane		000058-89-9				
mixed hexachlorocyclohexanes		000319-84-6				

WATER SOLUBILITY- 3							
relative to subcooled liquid							
NAME		water	at what	temp		data	
common chemical name	IUPAC #	cas # (1)	solubility	units	temp?	units	reference notes
cadmium		007440-43-9					
cadmium carbonate		000513-78-0					
cadmium chloride		010108-64-2					
cadmium oxide		001306-19-0					
cadmium sulfate		010124-36-4					
cadmium sulfide		001306-23-6					
elemental mercury		007439-97-6					
mercury oxide		021908-53-2					
mercuric chloride		007487-94-7					
monomethyl mercury chloride		000115-09-3					
dimethyl mercury		000593-74-8					
tetraethyl lead		000078-00-2					
tetramethyl lead		000075-74-1					
triethyl lead radical (1+ cation)		014570-15-1					
triethyl lead hydride		005224-23-7					
triethyl lead chloride		001067-14-7					
diethyl lead radical (2+ cation)		024952-65-6					
diethyl lead dihydride		081494-11-3					
diethyl lead dichloride		013231-90-8					
trimethyl lead radical (1+ cation)		014570-16-2					
trimethyl lead hydride		007442-13-9					
trimethyl lead chloride		001520-78-1					
dimethyl lead radical (2+ cation)		021774-13-0					
dimethyl lead dihydride		030691-92-0					
dimethyl lead dichloride		001520-77-0					
bis (tributyltin) oxide		000056-35-9					
tributyl tin		000688-75-3					
tributyltin fluoride		001983-10-4					
tributyltin chloride		001461-22-9					
tributyltin hydroxide		001067-97-6					
tributyltin naphthenate							
tris(tributylstanny) phosphate		013435-05-7					

WATER SOLUBILITY- 3							
relative to subcooled liquid							
NAME		water	at what	temp	reference	data	
common chemical name	IUPAC #	cas # (1)	solubility	units	temp?	units	
1,4-dichlorobenzene	000106-46-7		1.0653	mol/m3	25	deg C	5
1,2,3,4-tetrachlorobenzene	000634-66-2		0.0602	mol/m3	25	deg C	5
1,2,4,5-tetrachlorobenzene	000095-94-3		0.0784	mol/m3	25	deg C	5
1,2,3,5-tetrachlorobenzene	000634-90-2		0.0327	mol/m3	25	deg C	5
pentachlorobenzene	000608-93-5		0.0113	mol/m3	25	deg C	5
hexachlorobenzene	000118-74-1		0.00187	mol/m3	25	deg C	5
naphthalene	000091-20-3		855.92	mmol/m3	25	deg C	6
acenaphthene	000083-32-9		124.7	mmol/m3	25	deg C	6
acenaphthylene	000208-96-8		492.97	mmol/m3	25	deg C	6
fluorene	000086-73-7		90.816	mmol/m3	25	deg C	6
phenanthrene	000085-01-8		34.847	mmol/m3	25	deg C	6
anthracene	000120-12-7		19.65	mmol/m3	25	deg C	6
pyrene	000129-00-0		12.89	mmol/m3	25	deg C	6
fluoranthene	000206-44-0		8.41	mmol/m3	25	deg C	6
chrysene	000218-01-9		0.00876	mmol/m3	25	deg C	6
benz [ a ] anthracene	000056-55-3		1.045	mmol/m3	25	deg C	6
benzo [ b ] fluoranthene	000205-99-2		0.154	mmol/m3	25	deg C	6
benzo [ j ] fluoranthene	000205-82-3		0.246	mmol/m3	25	deg C	6
benzo [ k ] fluoranthene	000207-08-9		0.252	mmol/m3	25	deg C	6
benzo [ a ] pyrene	000050-32-8		0.459	mmol/m3	25	deg C	6
benzo [ e ] pyrene	000192-97-2		0.517	mmol/m3	25	deg C	6
perylene	000198-55-0		0.493	mmol/m3	25	deg C	6
benzo [ g,h,i ] perylene	000191-24-2		0.301	mmol/m3	25	deg C	6
dibenz [ a,h ] anthracene	000053-70-3		0.533	mmol/m3	25	deg C	6
indeno [ 1,2,3-c,d ] pyrene	000193-39-5		<i>not given in reference 6</i>				

WATER SOLUBILITY- 3						
relative to subcooled liquid						
NAME						
common chemical name	IUPAC #	cas # (1)	water solubility	at what units temp?	temp units	reference data notes
2,3,7,8-TCDD	001746-01-6		0.0352 mmol/m3	25 deg C	6	
1,2,3,7,8-PeCDD	040321-76-4		0.0159 mmol/m3	25 deg C	6	using value for 12347 PeCDD
1,2,3,4,7,8-HxCDD	039227-28-6		0.00321 mmol/m3	25 deg C	6	
1,2,3,6,7,8-HxCDD	057653-85-7		0.00321 mmol/m3	25 deg C	6	using value for 123478 HxCDD
1,2,3,7,8,9-HxCDD	019408-74-3		0.00321 mmol/m3	25 deg C	6	using value for 123478 HxCDD
1,2,3,4,6,7,8-HpCDD	035822-46-9		0.00133 mmol/m3	25 deg C	6	
OCDD	003268-87-9		0.00014 mmol/m3	25 deg C	6	
2,3,7,8-TCDF	051207-31-9		0.136 mmol/m3	25 deg C	6	
2,3,4,7,8-PeCDF	057117-31-4		0.0341 mmol/m3	25 deg C	6	
1,2,3,7,8-PeCDF	057117-41-6		0.0341 mmol/m3	25 deg C	6	using value for 23478 PeCDF
1,2,3,4,7,8-HxCDF	070648-26-9		2.12E-003 mmol/m3	25 deg C	6	
1,2,3,6,7,8-HxCDF	057117-44-9		5.27E-003 mmol/m3	25 deg C	6	
1,2,3,7,8,9-HxCDF	072918-21-9		3.70E-003 mmol/m3	25 deg C	6	using avg of values for 123478 HxCDF and 123678 HxCDF
2,3,4,6,7,8-HxCDF	060851-34-5		3.70E-003 mmol/m3	25 deg C	6	using avg of values for 123478 HxCDF and 123678 HxCDF
1,2,3,4,6,7,8-HpCDF	067562-39-4		4.03E-004 mmol/m3	25 deg C	6	
1,2,3,4,7,8,9-HpCDF	055673-89-7		4.03E-004 mmol/m3	25 deg C	6	using value for 1234678 HpCDF
OCDF	039001-02-0		5.27E-005 mmol/m3	25 deg C	6	

WATER SOLUBILITY- 3						
relative to subcooled liquid						
		water		at what	temp	data
common chemical name	IUPAC #	cas # (1)	solubility	units	temp?	units
biphenyl	0	000092-52-4	129.7	mmol/m3	25	deg C
2-PCB	1	002051-60-7	35.66	mmol/m3	25	deg C
3-PCB	2	002051-61-8	13.24	mmol/m3	25	deg C
4-PCB	3	002051-62-9	21.15	mmol/m3	25	deg C
count						
average						
standard deviation						
minimum						
maximum						
2,2'-PCB	4	013029-08-8	10.14	mmol/m3	25	deg C
2,3-PCB	5	016605-91-7	<i>not in reference 5</i>			
2,4-PCB	7	033284-50-3	5.51	mmol/m3	25	deg C
2,4'-PCB	8	034883-43-7	6.73	mmol/m3	25	deg C
2,5-PCB	9	034883-39-1	8.95	mmol/m3	25	deg C
2,6-PCB	10	033146-45-1	7.84	mmol/m3	25	deg C
3,3'-PCB	11	002050-67-1	1.738	mmol/m3	25	deg C
3,4-PCB	12	002974-92-7	<i>not in reference 5</i>			
3,5-PCB	14	034883-41-5	<i>not in reference 5</i>			
4,4'-PCB	15	002050-68-2	4.56	mmol/m3	25	deg C
count						
average						
standard deviation						
minimum						
maximum						

WATER SOLUBILITY- 3						
relative to subcooled liquid						
NAME			water	at what	temp	data
common chemical name	IUPAC #	cas # (1)	solubility	units	temp?	units
2,2',3-PCB	16	038444-78-9	-----	not in reference 5 -----		
2,2',5-PCB	18	037680-65-2	2.39	mmol/m3	25	deg C
2,3,3'-PCB	20	038444-84-7	-----	not in reference 5 -----		
2,3,4-PCB	21	055702-46-0	-----	not in reference 5 -----		
2,3',5-PCB	26	038444-85-8	1.387	mmol/m3	25	deg C
2,4,4'-PCB	28	007012-37-5	1.28	mmol/m3	25	deg C
2,4,5-PCB	29	015862-07-4	1.81	mmol/m3	25	deg C
2,4,6-PCB	30	035693-92-6	1.82	mmol/m3	25	deg C
2,4',5,-PCB	31	016606-02-3	-----	not in reference 5 -----		
2',3,4-PCB	33	038444-86-9	0.69	mmol/m3	25	deg C
3,3',4-PCB	35	037680-69-6	-----	not in reference 5 -----		
3,4,4'-PCB	37	038444-90-5	0.24	mmol/m3	25	deg C
count						
average						
standard deviation						
minimum						
maximum						
2,2',3,3'-PCB	40	038444-93-8	0.91	mmol/m3	25	deg C
2,2',3,5'-PCB	44	041464-39-5	0.565	mmol/m3	25	deg C
2,2',4,4'-PCB	47	002437-79-8	1.15	mmol/m3	25	deg C
2,2',4,5'-PCB	49	041464-40-8	0.133	mmol/m3	25	deg C
2,2',4,6-PCB	50	062796-65-0	-----	not in reference 5 -----		
2,2',4,6'-PCB	51	068194-04-7	-----	not in reference 5 -----		
2,2,5,5'-PCB	52	035693-99-3	0.42	mmol/m3	25	deg C
2,2,5,6'-PCB	53	041464-41-9	-----	not in reference 5 -----		
2,2,6,6'-PCB	54	015968-05-5	-----	not in reference 5 -----		
2,3,4,4'-PCB	60	033025-41-1	-----	not in reference 5 -----		
2,3,4,5-PCB	61	033284-53-6	0.314	mmol/m3	25	deg C
2,3,5,6-PCB	65	033284-54-7	-----	not in reference 5 -----		
2,3,4,4'-PCB	66	032598-10-0	1.3	mmol/m3	25	deg C
2,3',4',5-PCB	70	032598-11-1	-----	not in reference 5 -----		
2,4,4',6-PCB	75	032598-12-2	-----	not in reference 5 -----		
3,3',4,4'-PCB	77	032598-13-3	1.165	mmol/m3	25	deg C
3,3',5,5'-PCB	80	033284-52-5	0.0974	mmol/m3	25	deg C
3,4,4',5-PCB	81	070362-50-4	-----	not in reference 5 -----		
count						
average						
standard deviation						
minimum						
maximum						

WATER SOLUBILITY- 3						
relative to subcooled liquid						
		water	at what	temp	reference	data
common chemical name	IUPAC #	cas # (1)	solubility	units	temp?	units
2,2',3,3',5-PCB	83	060145-20-2	-----	not in reference 5	-----	-----
2,2',3,4,5-PCB	86	065510-45-4	0.337	mmol/m3	25 deg C	5
2,2',3,4,5'-PCB	87	038380-02-8	0.0927	mmol/m3	25 deg C	5
2,2',3,4,6-PCB	88	055215-17-3	0.202	mmol/m3	25 deg C	5
2,2',3,5,6-PCB	95	038379-99-6	-----	not in reference 5	-----	-----
2,2',4,4,5-PCB	99	038380-01-7	-----	not in reference 5	-----	-----
2,2',4,4,6-PCB	100	039485-83-1	-----	not in reference 5	-----	-----
2,2',4,5,5'-PCB	101	037680-73-2	0.0986	mmol/m3	25 deg C	5
2,2',4,6,6'-PCB	104	056558-16-8	0.3103	mmol/m3	25 deg C	5
2,3,3',4,4'-PCB	105	032598-14-4	-----	not in reference 5	-----	-----
2,3,3',4,6-PCB	110	038380-03-9	-----	not in reference 5	-----	-----
2,3,4,4',5-PCB	114	074472-37-0	-----	not in reference 5	-----	-----
2,3,4,5,6-PCB	116	018259-05-7	0.233	mmol/m3	25 deg C	5
2,3',4,4',5-PCB	118	031508-00-6	-----	not in reference 5	-----	-----
2,3,4,5,5'-PCB	124	070424-70-3	-----	not in reference 5	-----	-----
3,3',4,4',5-PCB	126	057465-28-8	-----	not in reference 5	-----	-----
count						
average						
standard deviation						
minimum						
maximum						
2,2',3,3',4,4'-PCB	128	038380-07-3	0.0286	mmol/m3	25 deg C	5
2,2',3,3',4,5-PCB	129	055215-18-4	0.0065	mmol/m3	25 deg C	5
2,2',3,3',5,6-PCB	134	052704-70-8	0.0061	mmol/m3	25 deg C	5
2,2',3,3',6,6'-PCB	136	038411-22-2	0.0161	mmol/m3	25 deg C	5
2,2',3,4,4',5'-PCB	138	035065-28-2	-----	not in reference 5	-----	-----
2,2',3,4,5,6-PCB	149	038380-04-0	-----	not in reference 5	-----	-----
2,2',4,4',5,5'-PCB	153	035065-27-1	0.0163	mmol/m3	25 deg C	5
2,2',4,4',6,6'-PCB	155	033979-03-2	0.042	mmol/m3	25 deg C	5
2,3,3',4,4',5-PCB	156	038380-08-4	-----	not in reference 5	-----	-----
2,3,3',4,4',5'-PCB	157	069782-90-7	-----	not in reference 5	-----	-----
2,3',4,4',5,5'-PCB	167	052663-72-6	-----	not in reference 5	-----	-----
3,3',4,4',5,5'-PCB	169	032774-16-6	-----	not in reference 5	-----	-----
count						
average						
standard deviation						
minimum						
maximum						

WATER SOLUBILITY- 3						
relative to subcooled liquid						
		water	at what	temp	data	
common chemical name	IUPAC #	cas # (1)	solubility	units	temp?	units
2,2',3,3',4,4',5-PCB	170	035065-30-6		-----	not in reference 5	
2,2',3,3',4,4',6-PCB	171	052663-71-5	0.046	mmol/m3	25 deg C	5
2,2',3,4,4',5,5'-PCB	180	035065-29-3		-----	not in reference 5	
2,2',3,4,5,5',6-PCB	185	052712-05-7	0.0191	mmol/m3	25 deg C	5
2,2',3,4',5,5',6-PCB	187	052663-68-0		-----	not in reference 5	
2,3,3',4,4',5,5'-PCB	189	039635-31-9		-----	not in reference 5	
count						
average						
standard deviation						
minimum						
maximum						
2,2',3,3',4,4',5,5'-PCB	194	035694-08-7	0.0098	mmol/m3	25 deg C	5
2,2',3,3',5,5',6,6'-PCB	202	002136-99-4	0.0158	mmol/m3	25 deg C	5
count						
average						
standard deviation						
minimum						
maximum						
2,2',3,3',4,4',5,5',6-PCB	206	040186-72-9	0.0146	mmol/m3	25 deg C	5
2,2',3,3',4,4',5,6,6'-PCB	207	052663-79-3		-----	not in reference 5	
2,2',3,3',4,5,5',6,6'-PCB	208	052663-77-1	0.00141	mmol/m3	25 deg C	5
count						
average						
standard deviation						
minimum						
maximum						
2,2',3,3',4,4',5,5',6,6'-PCB	209	002051-24-3	0.0144	mmol/m3	25 deg C	5

HENRY's LAW CONSTANT- 1							
NAME							
			Henry's Law Const for gas wet	Henry's dep estim	Law	at what temp	how
common chemical name	IUPAC #	cas # (1)	[atm m3/mol]	temp (K)	Constant	units	temp? units reference determined
octachlorostyrene	029082-74-4		1.30E-004	293.15	1.3E-004	atm m3/mol	20 deg C 58 experimental
4-bromophenyl phenyl ether	000101-55-3		1.02E-004	298.15	10.38	Pa m3/mol	25 deg C 7 calc'd from P/C
3,3'-dichlorobenzidine	000091-94-1		4.93E-008	298.15	5.0E-003	Pa m3/mol	25 deg C 8 calc'd from P/C
1,3-dinitropyrene	075321-20-9		5.62E-007	298.15			
1,6-dinitropyrene	042397-64-8		5.62E-007	298.15			
1,8-dinitropyrene	042397-65-9		5.62E-007	298.15			
2,7-dinitropyrene	117929-15-4		5.62E-007	298.15			
dinitropyrenes (mixed)	078432-19-6						
hexachloro-1,3-butadiene	000087-68-3		1.52E-002	298.15	1540	Pa m3/mol	25 deg C 7 calc'd P/C
4,4'-methylene bis(2-chloroaniline)	000101-14-4		4.00E-011	?	4.0E-011	atm m3/mol	temp not report 15
pentachlorophenol	000087-86-5		0.0000007797	298.15	0.079	Pa m3/mol	25 deg C 8 calc'd P/C
aldrin	000309-00-2		4.96E-004	?	4.960E-004	atm m3/mol	temp not report 51
dielein	000060-57-1		5.80E-005	?	5.8E-005	atm m3/mol	temp not report 51
p,p'-DDT	000050-29-3		5.13E-004	?	5.13E-004	atm m3/mol	temp not stated 62 a lot of other conflicting data in ref 52
p,p'-DDD	000072-54-8		2.16E-005	?	2.16E-005	atm m3/mol	temp not stated 62 a lot of other conflicting data in ref 52
p,p'-DDE	000072-55-9		6.80E-005	?	6.8E-005	atm m3/mol	temp not stated 62 a lot of other conflicting data in ref 52
heptachlor	000076-44-8		1.48E-003	?	1.48E-003	atm m3/mol	temp not stated 51 not stated
heptachlor epoxide	001024-57-3		3.20E-005	?	3.2E-005	atm m3/mol	temp not stated 51 not stated
methoxychlor	000072-43-5		1.58E-005	298.15	1.58E-005	atm m3/mol	25 deg C 28 estimated
mirex	002385-85-5		8.28E-003	293.15	839.37	Pa m3/mole	20 deg C 69
toxaphene	008001-35-2		6.00E-006	293.15	6.0E-006	atm m3/mol	20 deg C 57 experimental
endrin	000072-20-8		7.52E-006	?	7.52E-006	atm m3/mol	temp not report 45 calculated
alpha-hexachlorocyclohexane	000319-84-6		5.40E-006	?	0.0000054	atm m3/mol	temp not report 33, 37
beta-hexachlorocyclohexane	000319-85-7		4.50E-007	?	4.5E-007	atm m3/mol	temp not report 38, 39
delta-hexachlorocyclohexane	000319-86-8		2.10E-007	?	2.1E-007	atm m3/mol	temp not report 37, 40
gamma-hexachlorocyclohexane	000058-89-9		5.50E-006	?	0.0000055	atm m3/mol	temp not report 37, 41
mixed hexachlorocyclohexanes	000319-84-6						

HENRY's LAW CONSTANT- 1							
NAME							
common chemical name	IUPAC #	cas # (1)	[atm m3/mol]	Henry's Law Const for gas wet dep estim	Henry's Law	at what temp	how
cadmium	007440-43-9			no data			77
cadmium carbonate	000513-78-0			no data			77
cadmium chloride	010108-64-2			no data			77
cadmium oxide	001306-19-0			no data			77
cadmium sulfate	010124-36-4			no data			77
cadmium sulfide	001306-23-6			no data			77
elemental mercury	007439-97-6		5.66E-003				
mercury oxide	021908-53-2						
mercuric chloride	007487-94-7		1.40E-008				
monomethyl mercury chloride	000115-09-3						
dimethyl mercury	000593-74-8						
tetraethyl lead	000078-00-2		5.68E-001	297.15	5.68E-001 atm-m3/mo	24 deg C	85 experimental
tetramethyl lead	000075-74-1		8.79E-001	293.15	8.79E-001 atm-m3/mo	20 deg C	97 estimated based on expt'l Vp and estim'd Ws
triethyl lead radical (1+ cation)	014570-15-1						
triethyl lead hydride	005224-23-7						
triethyl lead chloride	001067-14-7						
diethyl lead radical (2+ cation)	024952-65-6						
diethyl lead dihydride	081494-11-3						
diethyl lead dichloride	013231-90-8						
trimethyl lead radical (1+ cation)	014570-16-2						
trimethyl lead hydride	007442-13-9						
trimethyl lead chloride	001520-78-1						
dimethyl lead radical (2+ cation)	021774-13-0						
dimethyl lead dihydride	030691-92-0						
dimethyl lead dichloride	001520-77-0						
bis (tributyltin) oxide	000056-35-9		1.25E-007	293.15			
tributyl tin	000688-75-3						
tributyltin fluoride	001983-10-4						
tributyltin chloride	001461-22-9						
tributyltin hydroxide	001067-97-6						
tributyltin naphthenate							
tris(tributylstanny) phosphate	013435-05-7						

HENRY's LAW CONSTANT- 1								
NAME								
			Henry's Law Const for gas wet	Henry's				
common chemical name	IUPAC #	cas # (1)	[atm m3/mol]	temp (K)	Constant	units	temp? units	reference how
1,4-dichlorobenzene	000106-46-7		1.58E-003	298.15	160	Pa m3/mol	25 deg C	5 calc'd P/C
1,2,3,4-tetrachlorobenzene	000634-66-2		1.42E-003	298.15	144	Pa m3/mol	25 deg C	5 calc'd P/C
1,2,4,5-tetrachlorobenzene	000095-94-3		1.20E-003	298.15	122	Pa m3/mol	25 deg C	5 calc'd P/C
1,2,3,5-tetrachlorobenzene	000634-90-2		5.80E-003	298.15	588	Pa m3/mol	25 deg C	5 calc'd P/C
pentachlorobenzene	000608-93-5		8.39E-004	298.15	85	Pa m3/mol	25 deg C	5 calc'd P/C
hexachlorobenzene	000118-74-1		1.29E-003	298.15	131	Pa m3/mol	25 deg C	5 calc'd P/C
naphthalene	000091-20-3		4.24E-004	298.15	43.01	Pa m3/mol	25 deg C	6 calc'd P/C
acenaphthene	000083-32-9		1.20E-004	298.15	12.17	Pa m3/mol	25 deg C	6 calc'd P/C
acenaphthylene	000208-96-8		8.29E-005	298.15	8.40	Pa m3/mol	25 deg C	6 calc'd P/C
fluorene	000086-73-7		7.77E-005	298.15	7.87	Pa m3/mol	25 deg C	6 calc'd P/C
phenanthrene	000085-01-8		3.20E-005	298.15	3.24	Pa m3/mol	25 deg C	6 calc'd P/C
anthracene	000120-12-7		3.91E-005	298.15	3.96	Pa m3/mol	25 deg C	6 calc'd P/C
pyrene	000129-00-0		9.08E-006	298.15	0.92	Pa m3/mol	25 deg C	6 calc'd P/C
floranthene	000206-44-0		1.02E-005	298.15	1.04	Pa m3/mol	25 deg C	6 calc'd P/C
chrysene	000218-01-9		1.05E-006	?	1.05E-006	atm m3/mol	temp not report	10 not reported
benz [ a ] anthracene	000056-55-3		5.73E-006	298.15	0.581	Pa m3/mol	25 deg C	6 calc'd P/C
benzo [ b ] fluoranthene	000205-99-2		1.22E-005	?	1.22E-005	atm m3/mol	temp not report	10 not reported
benzo [ j ] fluoranthene	000205-82-3		1.00E-006	?	1.00E-006	atm m3/mol	temp not report	13 not reported
benzo [ k ] fluoranthene	000207-08-9		1.58E-007	298.15	0.016	Pa m3/mol	25 deg C	6 calc'd P/C
benzo [ a ] pyrene	000050-32-8		4.54E-007	298.15	0.046	Pa m3/mol	25 deg C	6 calc'd P/C
benzo [ e ] pyrene	000192-97-2		1.97E-007	298.15	0.020	Pa m3/mol	25 deg C	6 calc'd P/C
perylene	000198-55-0		2.96E-008	298.15	0.003	Pa m3/mol	25 deg C	6 calc'd P/C
benzo [ g,h,i ] perylene	000191-24-2		7.40E-007	298.15	0.08	Pa m3/mol	25 deg C	6 calc'd P/C
dibenz [ a,h ] anthracene	000053-70-3		7.30E-008	?	7.30E-008	atm m3/mol	temp not report	10 not reported
indeno [ 1,2,3-c,d ] pyrene	000193-39-5		6.95E-008	?	6.95E-008	atm-m3/mol	temp not report	10 not reported

HENRY's LAW CONSTANT- 1									
NAME		Henry's Law Const for gas wet		Henry's dep estim		at what temp		how	
common chemical name	IUPAC #	cas # (1)	[atm m3/mol]	temp (K)	Constant	units	temp?	units	reference
									determined
2,3,7,8-TCDD	001746-01-6		3.29E-005	298.15	3.337	Pa m3/mol	25	deg C	6 not stated
1,2,3,7,8-PeCDD	040321-76-4		2.63E-006	298.15	0.266	Pa m3/mol	25	deg C	6 not stated
1,2,3,4,7,8-HxCDD	039227-28-6		1.07E-005	298.15	1.084	Pa m3/mol	25	deg C	6 not stated
1,2,3,6,7,8-HxCDD	057653-85-7		1.07E-005	298.15	1.084	Pa m3/mol	25	deg C	6 not stated
1,2,3,7,8,9-HxCDD	019408-74-3		1.07E-005	298.15	1.084	Pa m3/mol	25	deg C	6 not stated
1,2,3,4,6,7,8-HpCDD	035822-46-9		1.26E-005	298.15	1.273	Pa m3/mol	25	deg C	6 not stated
OCDD	003268-87-9		6.75E-006	298.15	0.684	Pa m3/mol	25	deg C	6 not stated
2,3,7,8-TCDF	051207-31-9		1.44E-005	298.15	1.461	Pa m3/mol	25	deg C	6 not stated
2,3,4,7,8-PeCDF	057117-31-4		4.98E-006	298.15	0.505	Pa m3/mol	25	deg C	6 not stated
1,2,3,7,8-PeCDF	057117-41-6		4.98E-006	298.15	0.505	Pa m3/mol	25	deg C	6 not stated
1,2,3,4,7,8-HxCDF	070648-26-9		1.43E-005	298.15	1.454	Pa m3/mol	25	deg C	6 not stated
1,2,3,6,7,8-HxCDF	057117-44-9		7.31E-006	298.15	0.741	Pa m3/mol	25	deg C	6 not stated
1,2,3,7,8,9-HxCDF	072918-21-9		1.08E-005	298.15	1.098	Pa m3/mol	25	deg C	6 not stated
2,3,4,6,7,8-HxCDF	060851-34-5		1.08E-005	298.15	1.098	Pa m3/mol	25	deg C	6 not stated
1,2,3,4,6,7,8-HpCDF	067562-39-4		1.41E-005	298.15	1.425	Pa m3/mol	25	deg C	6 not stated
1,2,3,4,7,8,9-HpCDF	055673-89-7		1.41E-005	298.15	1.425	Pa m3/mol	25	deg C	6 not stated
OCDF	039001-02-0		1.89E-006	298.15	0.191	Pa m3/mol	25	deg C	6 not stated

HENRY's LAW CONSTANT- 1								
NAME		Henry's Law Const for gas wet	Henry's dep estim	Law	at what temp	temp?	units	how
common chemical name	IUPAC #	cas # (1)	[atm m3/mol]	temp (K)	Constant	temp?	units	reference
biphenyl	0	000092-52-4	5.28E-004	298.15	53.5	Pa m3/mol	25 deg	C
2-PCB	1	002051-60-7	6.92E-004	298.15	70.1	Pa m3/mol	25 deg	C
3-PCB	2	002051-61-8	7.46E-004	298.15	75.55	Pa m3/mol	25 deg	C
4-PCB	3	002051-62-9	4.20E-004	298.15	42.56	Pa m3/mol	25 deg	C
count								
average								
standard deviation								
minimum								
maximum								
2,2'-PCB	4	013029-08-8	5.84E-004	298.15	59.17	Pa m3/mol	25 deg	C
2,3-PCB	5	016605-91-7						<i>not in reference 5</i>
2,4-PCB	7	033284-50-3	4.48E-004	298.15	45.39	Pa m3/mol	25 deg	C
2,4'-PCB	8	034883-43-7						<i>not in reference 5</i>
2,5-PCB	9	034883-39-1	1.98E-004	298.15	20.1	Pa m3/mol	25 deg	C
2,6-PCB	10	033146-45-1						<i>not in reference 5</i>
3,3'-PCB	11	002050-67-1	1.70E-004	298.15	17.26	Pa m3/mol	25 deg	C
3,4-PCB	12	002974-92-7						<i>not in reference 5</i>
3,5-PCB	14	034883-41-5						<i>not in reference 5</i>
4,4'-PCB	15	002050-68-2	1.68E-004	298.15	17	Pa m3/mol	25 deg	C
count								
average								
standard deviation								
minimum								
maximum								

HENRY's LAW CONSTANT- 1									
		Henry's Law Const for gas wet		Henry's					
		dep estim		Law		at what temp		how	
common chemical name	IUPAC #	cas # (1)	[atm m3/mol]	temp (K)	Constant	units	temp? units	reference	determined
2,2',3-PCB	16	038444-78-9						-----	not in reference 5 -----
2,2',5-PCB	18	037680-65-2	9.10E-004	298.15	92.21	Pa m3/mole	25 deg	C	calc'd P/C
2,3,3'-PCB	20	038444-84-7						-----	not in reference 5 -----
2,3,4-PCB	21	055702-46-0						-----	not in reference 5 -----
2,3',5-PCB	26	038444-85-8						-----	not in reference 5 -----
2,4,4'-PCB	28	007012-37-5						-----	not in reference 5 -----
2,4,5-PCB	29	015862-07-4	2.40E-004	298.15	24.29	Pa m3/mol	25 deg	C	calc'd P/C
2,4,6-PCB	30	035693-92-6	4.89E-004	298.15	49.51	Pa m3/mol	25 deg	C	calc'd P/C
2,4',5,-PCB	31	016606-02-3						-----	not in reference 5 -----
2',3,4-PCB	33	038444-86-9	4.31E-004	298.15	43.67	Pa m3/mol	25 deg	C	calc'd P/C
3,3',4-PCB	35	037680-69-6						-----	not in reference 5 -----
3,4,4'-PCB	37	038444-90-5						-----	not in reference 5 -----
count									
average									
standard deviation									
minimum									
maximum									
2,2',3,3'-PCB	40	038444-93-8	2.17E-004	298.15	21.94	Pa m3/mol	25 deg	C	calc'd P/C
2,2',3,5'-PCB	44	041464-39-5						-----	not in reference 5 -----
2,2',4,4'-PCB	47	002437-79-8	1.72E-004	298.15	17.38	Pa m3/mol	25 deg	C	calc'd P/C
2,2',4,5'-PCB	49	041464-40-8						-----	not in reference 5 -----
2,2',4,6-PCB	50	062796-65-0						-----	not in reference 5 -----
2,2',4,6'-PCB	51	068194-04-7						-----	not in reference 5 -----
2,2,5,5'-PCB	52	035693-99-3	4.70E-004	298.15	47.59	Pa m3/mol	25 deg	C	calc'd P/C
2,2,5,6'-PCB	53	041464-41-9						-----	not in reference 5 -----
2,2,6,6'-PCB	54	015968-05-5						-----	not in reference 5 -----
2,3,4,4'-PCB	60	033025-41-1						-----	not in reference 5 -----
2,3,4,5-PCB	61	033284-53-6						-----	not in reference 5 -----
2,3,5,6-PCB	65	033284-54-7						-----	not in reference 5 -----
2,3,4,4'-PCB	66	032598-10-0						-----	not in reference 5 -----
2,3',4',5-PCB	70	032598-11-1						-----	not in reference 5 -----
2,4,4',6-PCB	75	032598-12-2						-----	not in reference 5 -----
3,3',4,4'-PCB	77	032598-13-3	1.70E-005	298.15	1.72	Pa m3/mol	25 deg	C	calc'd P/C
3,3',5,5'-PCB	80	033284-52-5						-----	not in reference 5 -----
3,4,4',5-PCB	81	070362-50-4						-----	not in reference 5 -----
count									
average									
standard deviation									
minimum									
maximum									





HENRY's LAW CONSTANT- 1 (continued)							
common chemical name	IUPAC #	cas # (1)	Pa m3/mol	H calc'd	percent	calc	data
				from	diff of		
				P-liquid/ C-liquid	pressure basis	solubility basis	stated
						calc vs.	notes
octachlorostyrene	029082-74-4						
4-bromophenyl phenyl ether	000101-55-3		10.4	liquid	liquid		
3,3'-dichlorobenzidine	000091-94-1		4.58E-003	liquid	liquid		same for solid basis
1,3-dinitropyrene	075321-20-9		5.70E-002	solid	solid		
1,6-dinitropyrene	042397-64-8		5.70E-002	solid	solid		
1,8-dinitropyrene	042397-65-9		5.70E-002	solid	solid		
2,7-dinitropyrene	117929-15-4		5.70E-002	solid	solid		
dinitropyrenes (mixed)	078432-19-6						
hexachloro-1,3-butadiene	000087-68-3		1538	saturated	saturated		
4,4'-methylene bis(2-chloroaniline)	000101-14-4						
pentachlorophenol	000087-86-5		0.078	solid	solid		
aldrin	000309-00-2						
dielectron	000060-57-1						
p,p'-DDT	000050-29-3						
p,p'-DDD	000072-54-8						
p,p'-DDE	000072-55-9						
heptachlor	000076-44-8						
heptachlor epoxide	001024-57-3						
methoxychlor	000072-43-5						
mirex	002385-85-5						
toxaphene	008001-35-2						
endrin	000072-20-8						
alpha-hexachlorocyclohexane	000319-84-6					avg of two reported values	
beta-hexachlorocyclohexane	000319-85-7						
delta-hexachlorocyclohexane	000319-86-8						
gamma-hexachlorocyclohexane	000058-89-9					avg of two reported values	
mixed hexachlorocyclohexanes	000319-84-6						

HENRY's LAW CONSTANT- 1 (continued)							
common chemical name	IUPAC #	cas # (1)	H calc'd from P-liquid/ C-liquid	percent diff of basis stated	calc vs. for calc for calc	calc value	data notes
cadmium	007440-43-9						
cadmium carbonate	000513-78-0						
cadmium chloride	010108-64-2						
cadmium oxide	001306-19-0						
cadmium sulfate	010124-36-4						
cadmium sulfide	001306-23-6						
elemental mercury	007439-97-6	573.544711	liquid	liquid			
mercury oxide	021908-53-2						
mercuric chloride	007487-94-7	0.00142002	solid	solid	using estim	of Vp at 290 from V/P calc	
monomethyl mercury chloride	000115-09-3						
dimethyl mercury	000593-74-8						
tetraethyl lead	000078-00-2						
tetramethyl lead	000075-74-1	89106.0049					
triethyl lead radical (1+ cation)	014570-15-1						
triethyl lead hydride	005224-23-7						
triethyl lead chloride	001067-14-7						
diethyl lead radical (2+ cation)	024952-65-6						
diethyl lead dihydride	081494-11-3						
diethyl lead dichloride	013231-90-8						
trimethyl lead radical (1+ cation)	014570-16-2						
trimethyl lead hydride	007442-13-9						
trimethyl lead chloride	001520-78-1						
dimethyl lead radical (2+ cation)	021774-13-0						
dimethyl lead dihydride	030691-92-0						
dimethyl lead dichloride	001520-77-0						
bis (tributyltin) oxide	000056-35-9	0.01270552			Pa (g/mol)	m3/g	
tributyl tin	000688-75-3						
tributyltin fluoride	001983-10-4						
tributyltin chloride	001461-22-9						
tributyltin hydroxide	001067-97-6						
tributyltin naphthenate							
tris(tributylstanny) phosphate	013435-05-7						

HENRY's LAW CONSTANT- 1 (continued)							
common chemical name	IUPAC #	cas # (1)	Pa m3/mol	H calc'd	percent	calc	data
				from	diff of	solubility	calc vs.
				P-liquid/	pressure	stated	
				C-liquid	basis	value	notes
					basis	notes	notes
1,4-dichlorobenzene	000106-46-7		160	saturated	saturated		
1,2,3,4-tetrachlorobenzene	000634-66-2		144	saturated	saturated		
1,2,4,5-tetrachlorobenzene	000095-94-3		122	saturated	saturated		
1,2,3,5-tetrachlorobenzene	000634-90-2		587	saturated	saturated		
pentachlorobenzene	000608-93-5		85	saturated	saturated		
hexachlorobenzene	000118-74-1		131	saturated	saturated		
naphthalene	000091-20-3		4.30E+001	liquid	liquid	= solid basis	
acenaphthene	000083-32-9		1.22E+001	liquid	liquid	= solid basis	
acenaphthylene	000208-96-8		8.40E+000	liquid	liquid	= solid basis	
fluorene	000086-73-7		7.87E+000	liquid	liquid	= solid basis	
phenanthrene	000085-01-8		3.24E+000	liquid	liquid	= solid basis	
anthracene	000120-12-7		3.96E+000	liquid	liquid	= solid basis	
pyrene	000129-00-0		9.23E-001	liquid	liquid	= solid basis	
floranthene	000206-44-0		1.04E+000	liquid	liquid	= solid basis	
chrysene	000218-01-9		1.22E+001	liquid	liquid	no "solid" data	
benz [ a ] anthracene	000056-55-3		5.80E-001	liquid	liquid	= solid basis	
benzo [ b ] fluoranthene	000205-99-2						
benzo [ j ] fluoranthene	000205-82-3						
benzo [ k ] fluoranthene	000207-08-9		1.63E-002	liquid	liquid	= solid basis	
benzo [ a ] pyrene	000050-32-8		4.64E-002	liquid	liquid	= solid basis	
benzo [ e ] pyrene	000192-97-2		4.66E-002	liquid	liquid	= solid basis	
perylene	000198-55-0		8.81E-003	solid	solid		
benzo [ g,h,i ] perylene	000191-24-2		7.48E-002	liquid	liquid		
dibenz [ a,h ] anthracene	000053-70-3		1.72E-004	liquid	liquid	= solid basis	
indeno [ 1,2,3-c,d ] pyrene	000193-39-5						

<b>HENRY's LAW CONSTANT- 1 (continued)</b>							
common chemical name	IUPAC #	cas # (1)	Pa m3/mol	H calc'd	percent	calc	data
				from	diff of		
				P-liquid/ basis	solubility	calc vs.	
				C-liquid	basis	stated	
2,3,7,8-TCDD	001746-01-6	1.64430921	solid	solid	51% different because using different solid vapor pressure than Mackay		
1,2,3,7,8-PeCDD	040321-76-4	0.26586103	solid	solid	0%	using value for 12347 PeCDD	
1,2,3,4,7,8-HxCDD	039227-28-6	0.45132743	solid	solid	58%	?? why different?	
1,2,3,6,7,8-HxCDD	057653-85-7	0.45132743	solid	solid	58%	?? why different?	using value for 123478 HxCDD
1,2,3,7,8,9-HxCDD	019408-74-3	0.45132743	solid	solid	58%	?? why different?	using value for 123478 HxCDD
1,2,3,4,6,7,8-HpCDD	035822-46-9	0.13297872	solid	solid	90%	?? why different?	
OCDD	003268-87-9	0.68322981	solid	solid	0%	?? different when calc with liquid	
2,3,7,8-TCDF	051207-31-9	1.45985401	solid	solid	0%		
2,3,4,7,8-PeCDF	057117-31-4	0.50505051	solid	solid	0%		
1,2,3,7,8-PeCDF	057117-41-6	0.50505051	solid	solid	0%	using value for 23478 PeCDF	
1,2,3,4,7,8-HxCDF	070648-26-9	1.45454545	solid	solid	0%		
1,2,3,6,7,8-HxCDF	057117-44-9	0.74152542	solid	solid	0%		
1,2,3,7,8,9-HxCDF	072918-21-9	0.96820809	solid	solid	12%	using avg of values for 123478 HxCDF and 123678	
2,3,4,6,7,8-HxCDF	060851-34-5	0.96820809	solid	solid	12%	using avg of values for 123478 HxCDF and 123678	
1,2,3,4,6,7,8-HpCDF	067562-39-4	1.42424242	solid	solid	0%		
1,2,3,4,7,8,9-HpCDF	055673-89-7	1.87878788	solid	solid	32%	using value for 1234678 HpCDF	
OCDF	039001-02-0	0.19157088	solid	solid	0%		

HENRY's LAW CONSTANT- 1 (continued)								
common chemical name	IUPAC #	cas # (1)	Pa m3/mol	H calc'd	percent	calc vs.	calc	data
				from	diff of			
biphenyl	0	000092-52-4		P-liquid/	pressure	solubility		
2-PCB	1	002051-60-7		C-liquid	basis	stated		
3-PCB	2	002051-61-8			for calc	for calc	value	notes
4-PCB	3	002051-62-9						notes
count								
average								
standard deviation								
minimum								
maximum								
2,2'-PCB	4	013029-08-8						
2,3-PCB	5	016605-91-7						
2,4-PCB	7	033284-50-3						
2,4'-PCB	8	034883-43-7						
2,5-PCB	9	034883-39-1						
2,6-PCB	10	033146-45-1						
3,3'-PCB	11	002050-67-1						
3,4-PCB	12	002974-92-7						
3,5-PCB	14	034883-41-5						
4,4'-PCB	15	002050-68-2						
count								
average								
standard deviation								
minimum								
maximum								

HENRY's LAW CONSTANT- 1 (continued)									
common chemical name	IUPAC #	cas # (1)	Pa m3/mol	H calc'd	percent	solubility	calc vs.	calc	data
				from	diff of				
				P-liquid/	pressure				
				C-liquid	basis	basis	stated	notes	notes
2,2',3-PCB	16	038444-78-9							
2,2',5-PCB	18	037680-65-2							
2,3,3'-PCB	20	038444-84-7							
2,3,4-PCB	21	055702-46-0							
2,3',5-PCB	26	038444-85-8							
2,4,4'-PCB	28	007012-37-5							
2,4,5-PCB	29	015862-07-4							
2,4,6-PCB	30	035693-92-6							
2,4',5,-PCB	31	016606-02-3							
2',3,4-PCB	33	038444-86-9							
3,3',4-PCB	35	037680-69-6							
3,4,4'-PCB	37	038444-90-5							
count									
average									
standard deviation									
minimum									
maximum									
2,2',3,3'-PCB	40	038444-93-8							
2,2',3,5'-PCB	44	041464-39-5							
2,2',4,4'-PCB	47	002437-79-8							
2,2',4,5'-PCB	49	041464-40-8							
2,2',4,6-PCB	50	062796-65-0							
2,2',4,6'-PCB	51	068194-04-7							
2,2,5,5'-PCB	52	035693-99-3							
2,2,5,6'-PCB	53	041464-41-9							
2,2,6,6'-PCB	54	015968-05-5							
2,3,4,4'-PCB	60	033025-41-1							
2,3,4,5-PCB	61	033284-53-6							
2,3,5,6-PCB	65	033284-54-7							
2,3,4,4'-PCB	66	032598-10-0							
2,3',4',5-PCB	70	032598-11-1							
2,4,4',6-PCB	75	032598-12-2							
3,3',4,4'-PCB	77	032598-13-3							
3,3',5,5'-PCB	80	033284-52-5							
3,4,4',5-PCB	81	070362-50-4							
count									
average									
standard deviation									
minimum									
maximum									

HENRY's LAW CONSTANT- 1 (continued)								
common chemical name	IUPAC #	cas # (1)	Pa m3/mol	H calc'd	percent	calc vs.	calc	data
				from	P-liquid/ basis			
2,2',3,3',5-PCB	83	060145-20-2						
2,2',3,4,5-PCB	86	065510-45-4						
2,2',3,4,5'-PCB	87	038380-02-8						
2,2',3,4,6-PCB	88	055215-17-3						
2,2',3,5,6-PCB	95	038379-99-6						
2,2',4,4,5-PCB	99	038380-01-7						
2,2',4,4',6-PCB	100	039485-83-1						
2,2',4,5,5'-PCB	101	037680-73-2						
2,2',4,6,6'-PCB	104	056558-16-8						
2,3,3',4,4'-PCB	105	032598-14-4						
2,3,3',4,6-PCB	110	038380-03-9						
2,3,4,4',5-PCB	114	074472-37-0						
2,3,4,5,6-PCB	116	018259-05-7						
2,3',4,4',5-PCB	118	031508-00-6						
2',3,4,5,5'-PCB	124	070424-70-3						
3,3',4,4',5-PCB	126	057465-28-8						
count								
average								
standard deviation								
minimum								
maximum								
2,2',3,3',4,4'-PCB	128	038380-07-3						
2,2',3,3',4,5-PCB	129	055215-18-4						
2,2',3,3',5,6-PCB	134	052704-70-8						
2,2',3,3',6,6'-PCB	136	038411-22-2						
2,2',3,4,4',5-PCB	138	035065-28-2						
2,2',3,4',5,6-PCB	149	038380-04-0						
2,2',4,4',5,5'-PCB	153	035065-27-1						
2,2',4,4',6,6'-PCB	155	033979-03-2						
2,3,3',4,4',5-PCB	156	038380-08-4						
2,3,3',4,4',5'-PCB	157	069782-90-7						
2,3',4,4',5,5'-PCB	167	052663-72-6						
3,3',4,4',5,5'-PCB	169	032774-16-6						
count								
average								
standard deviation								
minimum								
maximum								

HENRY's LAW CONSTANT- 1 (continued)								
common chemical name	IUPAC #	cas # (1)	Pa m3/mol	H calc'd	percent	calc vs.	calc	data
				from	diff of			
			P-liquid/ C-liquid	pressure basis	solubility basis	calc vs.	calc	data
2,2',3,3',4,4',5-PCB	170	035065-30-6						
2,2',3,3',4,4',6-PCB	171	052663-71-5						
2,2',3,4,4',5,5'-PCB	180	035065-29-3						
2,2',3,4,5,5',6-PCB	185	052712-05-7						
2,2',3,4,5,5',6-PCB	187	052663-68-0						
2,3,3',4,4',5,5'-PCB	189	039635-31-9						
count								
average								
standard deviation								
minimum								
maximum								
2,2',3,3',4,4',5,5'-PCB	194	035694-08-7						
2,2',3,3',5,5',6,6'-PCB	202	002136-99-4						
count								
average								
standard deviation								
minimum								
maximum								
2,2',3,3',4,4',5,5',6-PCB	206	040186-72-9						
2,2',3,3',4,4',5,6,6'-PCB	207	052663-79-3						
2,2',3,3',4,5,5',6,6'-PCB	208	052663-77-1						
count								
average								
standard deviation								
minimum								
maximum								
2,2',3,3',4,4',5,5',6,6'-PCB	209	002051-24-3						

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Note: this last 310C @ 10mmHg is not a "real" boiling point, e.g., at atmospheric pressure;  
it is a boiling point at a much reduced pressure  
However, this data was used to make an estimate of the "real" boiling point, i.e., the temperature at which  
the liquid vapor pressure equals one atmosphere (detailed calc shown on another sheet)

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As a basis, used the 145 deg C at 2 mmHg boiling point, given in ref 85 and ref 48  
Note: this 145 C @ 2 mmHg is not a "real" boiling point, e.g., at atmospheric pressure;  
it is a boiling point at a much reduced pressure  
However, this data was used to make an estimate of the "real" boiling point, i.e., the temperature at which  
the liquid vapor pressure equals one atmosphere (detailed calc shown on another sheet)  
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## **Appendix B.**

### **Estimation Methods Used for Physical Chemical Properties**

- B.1. Estimation of Boiling Temperature ( $T_b$ ) at 1 atm pressure  
(when  $T_b$  given at a pressure other than 1 atm)
- B.2. Estimate of Boiling Temperature and Melting Temperature for Octachlorostyrene
- B.3. Estimation of Physical Properties for Dinitropyrenes
- B.4. Methodology Used to Estimate Boiling Temperature When No Data Were Available  
(based on Regression Between Melting Temperature and Boiling Temperature for Other Compounds)

## **Appendix B.1.**

**Estimation of Boiling Temperature ( $T_b$ ) at 1 atm pressure  
(when  $T_b$  given at a pressure other than 1 atm)**

Zeroth Order Estimation Procedure for Boiling Temperature  
When  $T_b$  given for a different pressure than Atmospheric

===== : ===== =====: ===== =====

Basis of Calculation:

===== : ===== =====: ===== =====

Suppose  $T_b'$  given at a different pressure than atmospheric

Suppose this pressure is  $P_b$

What is the  $T_b$  at atmospheric pressure, i.e., the normal boiling point?

Use the Clausius Clapyron equation to estimate this...

$$\ln(P_b/P_{atm}) = 84 * T_b / R (1/T_b' - 1/T_b)$$

This equation makes use of Troutons Rule, in which the enthalpy of vaporization can be approximately estimated by:

$$\Delta H / T_{boil} = 84 \text{ J/(mol deg K)}$$

Solving the above equation for  $T_b$  (in terms of  $T_b'$  and  $P_b$ ), one gets:

$$T_b = T_b' (K) * [ 1 - (R / 84) \ln (P_b / 1 \text{ atm}) ]$$

$$\text{where } R = 8.3144 \text{ J/(mol deg K)}$$

parameter	Benz(e)Pyrene				Aldrin			
	value	units	ref	notes	value	units	ref	notes
T boil at non std pres. = Tb'	584.15	deg K		86	418.15	deg K		85
Non std pressure for Tb'	10	mm Hg		86	2	mm Hg		85
R / 84	0.0990	dimensionless			0.0990	dimensionless		
ln (Pb / 1 atm)	-4.3307	dimensionless			-5.9402	dimensionless		
T-boil estimate at 1 atm	834.55	deg K			664.01	deg K		
Independent Estm of T-boil at 1 atm								

parameter	p,p'-DDD				Heptachlor			
	value	units	ref	notes	value	units	ref	notes
T boil at non std pres. = Tb'	466.15	deg K		60	418.15	deg K	?	
Non std pressure for Tb'	1	mm Hg		60	1.5	mm Hg	?	
R / 84	0.0990	dimensionless			0.0990	dimensionless		
ln (Pb / 1 atm)	-6.6333	dimensionless			-6.2279	dimensionless		
T-boil estimate at 1 atm	772.21	deg K			675.91	deg K		
Independent Estm of T-boil at 1 atm	623.15	deg K		not that close to the estimate above (?) Use this new value in V/P calculation	85	583.15	deg K	not that close to the estimate above (?) Use this new value in V/P calculation

parameter	Beta Hexachlorocyclohexane				Delta Hexachlorocyclohexane			
	value	units	ref	notes	value	units	ref	notes
T boil at non std pres. = Tb'	333.15	deg K			333.15	deg K		
Non std pressure for Tb'	0.5	mm Hg			0.36	mm Hg		
R / 84	0.0990	dimensionless			0.0990	dimensionless		
ln (Pb / 1 atm)	-7.3265	dimensionless			-7.6550	dimensionless		
T-boil estimate at 1 atm	574.74	deg K			585.58	deg K		
Independent Estm of T-boil at 1 atm								

parameter	Bis (Tributyltin) Oxide (TBTO)				Tetramethyl Lead (TML)			
	value	units	ref	notes	value	units	ref	notes
T boil at non std pres. = Tb'	527.15	deg K			383.15	deg K		
Non std pressure for Tb'	50	mm Hg			10	mm Hg		
R / 84	0.0990	dimensionless			0.0990	dimensionless		
ln (Pb / 1 atm)	-2.7213	dimensionless			-4.3307	dimensionless		
T-boil estimate at 1 atm	669.14	deg K			547.39	deg K		
Independent Estm of T-boil at 1 atm								

**Appendix B.2.**

**Estimate of Boiling Temperature and Melting Temperature  
for Octachlorostyrene**

Is there a relatively simple relationship between Parent Compounds and Fully Chlorinated Derivatives for Boiling Point and Melting Point?																														
parent compound	fully chlorinated compound	boiling			boiling			boiling			melting			melting																
		temp of parent compound	deg C	deg K ref	temp of fully-Cl'd compound	deg C	deg K ref	temp of fully-Cl'd predicted by regression	deg K	percent error	temp of parent compound	deg C	deg K ref	temp of fully-Cl'd compound	deg C	deg K ref	temp of fully-Cl'd predicted by regression	deg K	percent error											
styrene	octachlorostyrene	145	418	88	?	?		652		-31	242.15	88	?	?		423														
3-cyclohexanone	octachloro-3-cyclohexanone	155	429	88	?	?	88	663		-31	242	88	104	377	88	423	12%													
propane	octachloropropane	-42	231	88	?	?	88	462		-188	86	88	160	433	88	276	-36%													
1,5-hexadiene	decachloro-1,5-hexadiene	59	333	88	?	?	88	565		-141	132	88	49	322	88	320	-1%													
biphenyl	decachloro-PCB	255	528	5	?	?		764		71	344	5	306	579	5	519	-10%													
naphthalene	octachloronaphthalene	218	491	85	?	?		727		80	353	85	198	471	88	528	12%													
styrene	octachlorostyrene	145	418	88				652		-31	242.15	88				423														
methane	carbon tetrachloride	-162	112	88	77	350	88	340	-3%	-182	91	88	-23	250	88	281	12%													
ethylene	tetrachloroethylene	-104	169	88	121	394	88	399	1%	-169	104	88	-22	251	88	294	17%													
1,3-butadiene	hexachlorobutadiene	-4	269	88	215	488	85	500	2%	-109	164	88	-21	252	85	350	39%													
cyclopentene	octachlorocyclopentene	44	317	88	283	556	88	550	-1%	-135	138	88	40	313	88	325	4%													
benzene	hexachlorobenzene	80	353	5	319	592	85	586	-1%	6	279	5	230	503	5	457	-9%													
cyclohexane	avg for HCH's	81	354	88	306	579	85	587	1%	7	280	88	182	455	85	458	1%													
dibenzo-p-dioxin	OCDD	284	557	6	510	783	6	793	1%	123	396	6	322	595	6	568	-5%													
dibenofuran	OCDF	287	560	6	537	810	6	797	-2%	87	360	6	258	531	6	533	0%													
phenol	pentachlorophenol	182	455	88	310	583	85	690	18%	41	314	88	174	447	85	491	10%													
cyclohexane	beta-HCH	81	354	88	?	?		587		7	280	88	315	588	85	458	-22%													
cyclohexane	delta-HCH	81	354	88	?	?		587		7	280	88	142	415	85	458	10%													
cyclohexane	alpha-HCH	81	354	88	288	561	85	587	5%	7	280	88	160	433	85	458	6%													
cyclohexane	gamma-HCH	81	354	88	323	597	85	587	-2%	7	280	88	113	386	85	458	19%													
	average for HCH's	81	354	88	306	579	85	587	1%	7	280	88	182	455	85	458	1%													
<hr/>																														
<b>Regression Output for Boiling Temperature</b>																														
Constant		226.7086								Constant		195.8783																		
Std Err of Y Est		10.6820								Std Err of Y Est		66.7442																		
R Squared		0.9964								R Squared		0.7372																		
No. of Observations		8								No. of Observations		13																		
Degrees of Freedom		6								Degrees of Freedom		11																		
X Coefficient(s)		1.0180								X Coefficient(s)		0.9386																		
Std Err of Coef.		0.0250								Std Err of Coef.		0.1690																		
<hr/>																														
<b>Regression Output for Melting Temperature</b>																														
Constant		195.8783								Constant		195.8783																		
Std Err of Y Est		66.7442								Std Err of Y Est		66.7442																		
R Squared		0.7372								R Squared		0.7372																		
No. of Observations		13								No. of Observations		13																		
Degrees of Freedom		11								Degrees of Freedom		11																		
X Coefficient(s)		0.9386								X Coefficient(s)		0.9386																		
Std Err of Coef.		0.1690								Std Err of Coef.		0.1690																		

Notes:

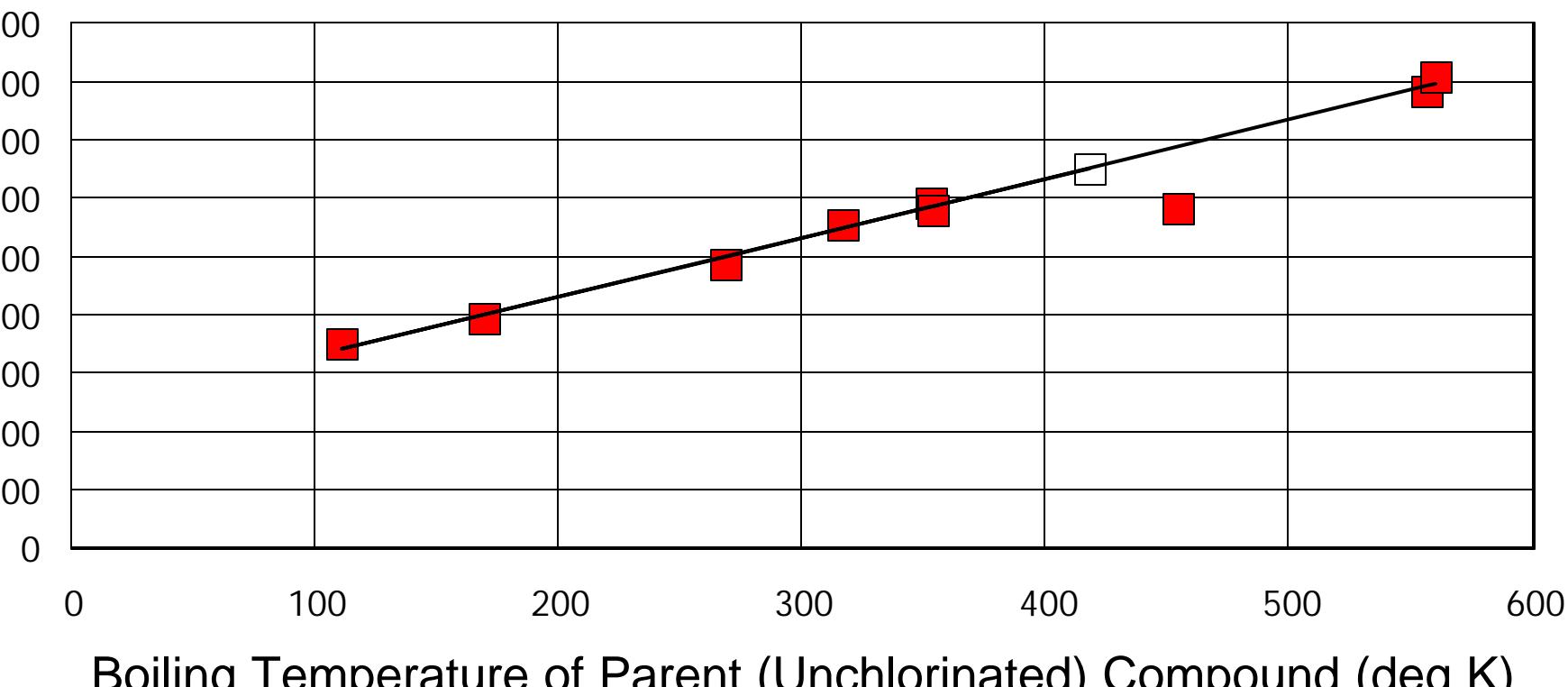
Phenol/Pentachlorophenol not included in regression; this pair seemed to be an outlier

Shaded data were included in regression

The purpose of this exercise was to crudely estimate physical properties of octachlorostyrene

Boiling Temperature of Fully Chlorinated Derivative (deg K)

### Boiling Point of a Series of Parent Compounds Compared With That of Their Fully Chlorinated Derivatives

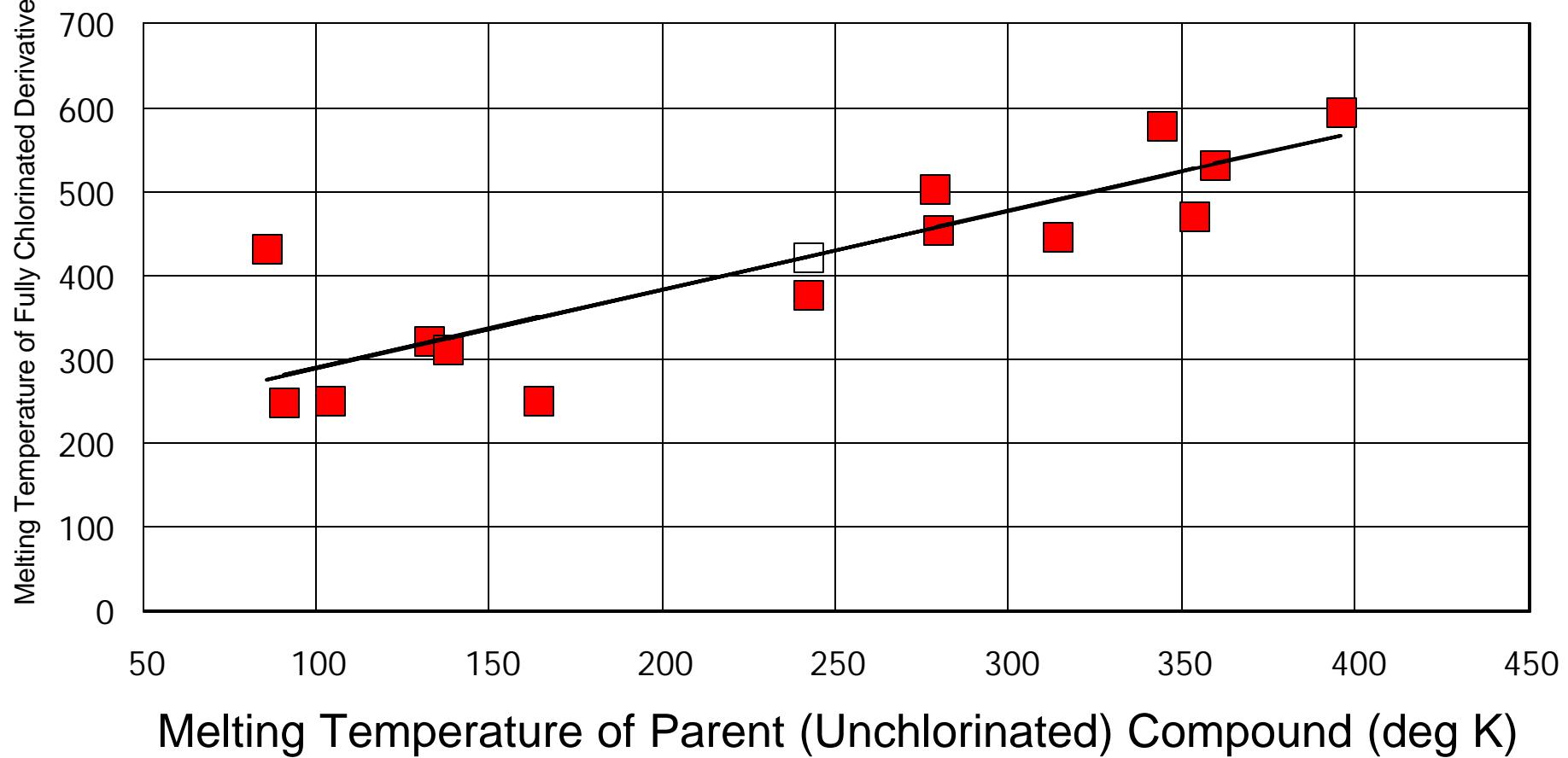


Boiling Temperature of Parent (Unchlorinated) Compound (deg K)

■ Matched Pairs (see tabular data) — linear regression □ Styrene / Octachlorostyrene

(outlier is phenol / pentachlorophenol pair; this pair was excluded in forming the regression)

Metling Point of a Series of Parent Compounds Compared  
With That of Their Fully Chlorinated Derivatives



■ Matched Pairs (see tabular data) — linear regression □ Styrene / Octachlorostyrene

**Appendix B.3.**

**Estimation of Physical Properties for Dinitropyrenes**

all references equal 88, unless stated  
 ref 88 = CRC Properties of Organic Compounds,  
 Personal Edition CD ROM, 1996

Some Physical Property Data for a Series of Compounds, with Parent Compounds  
 compared with Nitro- and Dinitro- substituted Derivatives

TYPE	CHEMICAL IDENTITY DATA			BOILING TEMPERATURE DATA										
	compound	cas #	molecular weight	Melt Temp		Boil Temp @ 1 atm			Boil Temp @ other pressure 1			Boil Temp @ other pressure 2		
				deg C	ref	deg C	ref	notes	deg C	mm Hg	ref	deg C	mm Hg	ref
parent	Benzene	71-43-2	78.11	6		80								
+ 1 nitro	Benzene, nitro-	98-95-3	123.11	6		211								
+2 nitro's	Benzene, 1,2-dinitro-	528-29-0	168.11	119		318			194	30				
+2 nitro's	Benzene, 1,3-dinitro-	99-65-0	168.11	90		291			167	14				
+2 nitro's	Benzene, 1,4-dinitro-	100-25-4	168.11	174		297			183	34				
parent	Naphthalene	91-20-3	128.17	80		218								
+ 1 nitro	Naphthalene, 1-nitro-	86-57-7	173.17	61					180	14				
+ 1 nitro	Naphthalene, 2-nitro-	581-89-5	173.17	79		314			165	15				
+2 nitro's	Naphthalene, 1,2-dinitro-	24934-47-2	218.17	163										
+2 nitro's	Naphthalene, 1,3-dinitro-	606-37-1	218.17	148		sublimates								
+2 nitro's	Naphthalene, 1,4-dinitro-	6921-26-2	218.17	133										
+2 nitro's	Naphthalene, 1,5-dinitro-	605-71-0	218.17	219		sublimates								
+2 nitro's	Naphthalene, 1,8-dinitro-	602-38-0	218.17	173		445	decompose							
+2 nitro's	Naphthalene, 2,3-dinitro-	1875-63-4	218.17	174										
+2 nitro's	Naphthalene, 2,7-dinitro-	24824-27-9	218.17	234										

all references equal 88, unless stated  
 ref 88 = CRC Properties of Organic Compounds,  
 Personal Edition CD ROM, 1996

Some Physical Property Data for a Series of Compounds, with Parent Compounds  
 compared with Nitro- and Dinitro- substituted Derivatives

TYPE	CHEMICAL IDENTITY DATA			BOILING TEMPERATURE DATA										
	compound	cas #	molecular weight	Melt Temp		Boil Temp @ 1 atm			Boil Temp @ other pressure 1			Boil Temp @ other pressure 2		
				deg C	ref	deg C	ref	notes	deg C	mm Hg	ref	deg C	mm Hg	ref
parent	1,1'-Biphenyl	92-52-4	154.21	69		256								
+ 1 nitro	1,1'-Biphenyl, 2-nitro-	86-00-0	199.21	37		320								
+ 1 nitro	1,1'-Biphenyl, 3-nitro-	2113-58-8	199.21	62					227	35		143	9	
+ 1 nitro	1,1'-Biphenyl, 4-nitro-	92-93-3	199.21	114		340								
+2 nitro's	1,1'-Biphenyl, 2,2'-dinitro-	2436-96-6	244.21	126		305								
+2 nitro's	1,1'-Biphenyl, 2,3'-dinitro-	7391-72-2	244.21	119										
+2 nitro's	1,1'-Biphenyl, 2,4'-dinitro-	608-81-5	244.21	94										
+2 nitro's	1,1'-Biphenyl, 3,3'-dinitro-	958-96-3	244.21	201										
+2 nitro's	1,1'-Biphenyl, 3,4'-dinitro-	6311-43-9	244.21	189										
+2 nitro's	1,1'-Biphenyl, 4,4'-dinitro-	1528-74-1	244.21	242										
parent	Dibenzofuran	132-64-9	168.19	87		287								
+ 1 nitro	Dibenzofuran, 1-nitro-	87812-99-5	213.19	121										
+ 1 nitro	Dibenzofuran, 3-nitro-	5410-97-9	213.19	182					182.5	3				
+ 1 nitro	Dibenzofuran, 4-nitro-	86607-81-0	213.19	139					197.5	15				
+2 nitro's	Dibenzofuran, 2,7-dinitro-	5408-55-9	258.19	256										
parent	Acenaphthene	83-32-9	154.21	93		279								
+ 1 nitro	Acenaphthene, 3-nitro-	3807-77-0	199.21	151.5										
+ 1 nitro	Acenaphthene, 5-nitro-	602-87-9	199.21	103.5										
+2 nitro's	Acenaphthene, 5,6-dinitro-	4406-87-5	244.21	223										

all references equal 88, unless stated  
 ref 88 = CRC Properties of Organic Compounds,  
 Personal Edition CD ROM, 1996

Some Physical Property Data for a Series of Compounds, with Parent Compounds  
 compared with Nitro- and Dinitro- substituted Derivatives

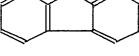
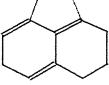
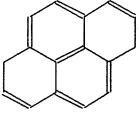
TYPE	compound	cas #	molecular weight	VAPOR PRESSURE DATA															
				Vp: -25 C		Vp: 0 C		Vp: 25 C		Vp: 50 C		Vp: 75 C		Vp: 100 C		Vp: 125 C		Vp: 150 C	
				Vp kPa	ref	Vp kPa	ref	Vp kPa	ref	Vp kPa	ref	Vp kPa	ref	Vp kPa	ref	Vp kPa	ref		
parent	Benzene	71-43-2	78.11	0.485		3.29		12.7		36.2		86.4		180		338		583	
+ 1 nitro	Benzene, nitro-	98-95-3	123.11					0.03										18.8	
+2 nitro's	Benzene, 1,2-dinitro-	528-29-0	168.11																
+2 nitro's	Benzene, 1,3-dinitro-	99-65-0	168.11																
+2 nitro's	Benzene, 1,4-dinitro-	100-25-4	168.11																
parent	Naphthalene	91-20-3	128.17					0.011				0.768		2.5		6.84		16.2	
+ 1 nitro	Naphthalene, 1-nitro-	86-57-7	173.17																
+ 1 nitro	Naphthalene, 2-nitro-	581-89-5	173.17																
+2 nitro's	Naphthalene, 1,2-dinitro-	24934-47-2	218.17																
+2 nitro's	Naphthalene, 1,3-dinitro-	606-37-1	218.17																
+2 nitro's	Naphthalene, 1,4-dinitro-	6921-26-2	218.17																
+2 nitro's	Naphthalene, 1,5-dinitro-	605-71-0	218.17																
+2 nitro's	Naphthalene, 1,8-dinitro-	602-38-0	218.17																
+2 nitro's	Naphthalene, 2,3-dinitro-	1875-63-4	218.17																
+2 nitro's	Naphthalene, 2,7-dinitro-	24824-27-9	218.17																

all references equal 88, unless stated  
 ref 88 = CRC Properties of Organic Compounds,  
 Personal Edition CD ROM, 1996

Some Physical Property Data for a Series of Compounds, with Parent Compounds  
 compared with Nitro- and Dinitro- substituted Derivatives

TYPE	compound	cas #	molecular weight	VAPOR PRESSURE DATA									
				Vp: -25 C		Vp: 0 C		Vp: 25 C		Vp: 50 C		Vp: 75 C	
				Vp kPa	ref	Vp kPa	ref	Vp kPa	ref	Vp kPa	ref	Vp kPa	ref
parent	1,1'-Biphenyl	92-52-4	154.21							0.149		0.586	
+ 1 nitro	1,1'-Biphenyl, 2-nitro-	86-00-0	199.21									1.87	
+ 1 nitro	1,1'-Biphenyl, 3-nitro-	2113-58-8	199.21										
+ 1 nitro	1,1'-Biphenyl, 4-nitro-	92-93-3	199.21										
+2 nitro's	1,1'-Biphenyl, 2,2'-dinitro-	2436-96-6	244.21										
+2 nitro's	1,1'-Biphenyl, 2,3'-dinitro-	7391-72-2	244.21										
+2 nitro's	1,1'-Biphenyl, 2,4'-dinitro-	608-81-5	244.21										
+2 nitro's	1,1'-Biphenyl, 3,3'-dinitro-	958-96-3	244.21										
+2 nitro's	1,1'-Biphenyl, 3,4'-dinitro-	6311-43-9	244.21										
+2 nitro's	1,1'-Biphenyl, 4,4'-dinitro-	1528-74-1	244.21										
parent	Dibenzofuran	132-64-9	168.19										
+ 1 nitro	Dibenzofuran, 1-nitro-	87812-99-5	213.19										
+ 1 nitro	Dibenzofuran, 3-nitro-	5410-97-9	213.19										
+ 1 nitro	Dibenzofuran, 4-nitro-	86607-81-0	213.19										
+2 nitro's	Dibenzofuran, 2,7-dinitro-	5408-55-9	258.19										
parent	Acenaphthene	83-32-9	154.21							0.281		0.949	
+ 1 nitro	Acenaphthene, 3-nitro-	3807-77-0	199.21										
+ 1 nitro	Acenaphthene, 5-nitro-	602-87-9	199.21										
+2 nitro's	Acenaphthene, 5,6-dinitro-	4406-87-5	244.21										

**Summary of Data Trends for: Parent Compounds, “+ 1 nitro group”, “+ 2 nitro groups”**  
 (can we make an educated guess at property value(s) for dinitropyrenes?)

Parent Compound	Molecular Weight of Parent	Structure of Parent	Melting Temperature	Boiling Temperature	Vapor Pressure
benzene	78		parent ~ nitro << dinitro  parent: 279 deg K	parent << nitro << dinitro  parent: 353 deg K	parent >> nitro <i>no data for dinitro</i>
naphthalene	128		parent ~ nitro << dinitro  parent: 353 deg K	parent << nitro << dinitro <i>but, not much data...;</i> <i>&amp; some dinitro cmpnds sublimate or decompose</i> parent: 491 deg K	? <i>no data for nitro/dinitro</i>
biphenyl	154		parent ~ nitro << dinitro  parent: 342 deg K	parent < nitro ~ dinitro <i>but, not much data...</i>  parent: 529 deg K	? <i>no data for nitro/dinitro</i>
dibenzofuran	168		parent << nitro << dinitro  parent: 360 deg K	? <i>no data for nitro/dinitro</i>  parent: 560 deg K	? <i>no data for nitro/dinitro</i>
acenaphthene	154		parent < nitro << dinitro  parent = 366 deg K	? <i>no data for nitro/dinitro</i>  parent: 552 deg K	? <i>no data for nitro/dinitro</i>
pyrene	202		parent = 424 deg K	parent = 677 deg K	

Estimation of Vapor Pressure, Using "Method 2" in: Lyman, W., 1982, "Vapor Pressure," in Handbook of Chemical Property Estimation Methods										
Chemical Properties of Pyrene and Dinitropyrene										
Parameter	Pyrene					Dinitropyrene				
	Type	Units	Value	Units	Ref	Notes	Value	Units	Ref	Notes
Tb: Boiling Temp	Data	deg K	677.15	deg K	88		727.15	deg K	88	crude: pyrene+50 C
Kf (from Table 14.4 or 14.5) (?)	Data	dimensionless	1	dimensionless	90	???	1.05	dimensionless	90	???
Temperature	User Specified	deg K	298.15	deg K			298.15	deg K		
Tpb = T/Tb	Calc	dimensionless	0.44	dimensionless			0.41	dimensionless		
Phys State for Estm: "solid" or "liquid"	Specified	text	solid				solid			
m	Data, based on Tpb	dimensionless	1.19	dimensionless	90		1.19	dimensionless	90	
R = gas constant	Constant	cal/mol K	1.987	cal /mol K			1.987	cal /mol K		
delta Hv <sub>b</sub> / Tb =	Calc: eqn 14-16	cal /mol K	21.7	cal /mol K			22.9	cal /mol K		
heat of vaporization at the normal boiling point, divided by the normal boiling point; this equals the entropy of vaporization at the normal boiling point = = Kf (8.75 + R ln Tb)										
delta Z <sub>b</sub> =	Estimated	dimensionless	0.97	dimensionless	90		0.97	dimensionless	90	
compressibility factor at normal boiling point										
factor1 in eqn 14-20	Calc: eqn 14-20	dimensionless	11.3	dimensionless			11.9	dimensionless		
factor2 in eqn 14-20	Calc: eqn 14-20	dimensionless	1	dimensionless			1	dimensionless		
factor3 in eqn 14-20	Calc: eqn 14-20	dimensionless	-4.86	dimensionless			-5.39	dimensionless		
factor4 in eqn 14-20	Calc: eqn 14-20	dimensionless	2.2517903903	dimensionless			2.4604847777	dimensionless		
In P <sub>vp</sub> from equation 14-20	Calc: eqn 14-20	dimensionless	-18.12142957	dimensionless			-22.9672106615	dimensionless		
P <sub>vp</sub>	Vapor Pressure	atm	1.35E-008	atm			1.06E-010	atm		
P <sub>vp</sub>	Vapor Pressure	mm Hg	1.03E-005	mm Hg			8.06E-008	mm Hg		
P <sub>vp</sub>	Vapor Pressure	Pa	1.37E-003	Pa			1.07E-005	Pa		
P <sub>vp</sub>	Vapor Pressure -- "Literature Value"	mm Hg	2.45E-006	mm Hg @25C	85	within an order of magnitude				
	Corrected for Ratio of Literature									
P <sub>vp</sub>	Value for Parent Compound to Estimated Value for Parent Compound	mm Hg					1.93E-008	mm Hg @25C		

Some Water Solubility Data for a Series of Compounds, with Parent Compounds compared with Nitro- and Dinitro- substituted Derivatives

all references equal 97, unless stated

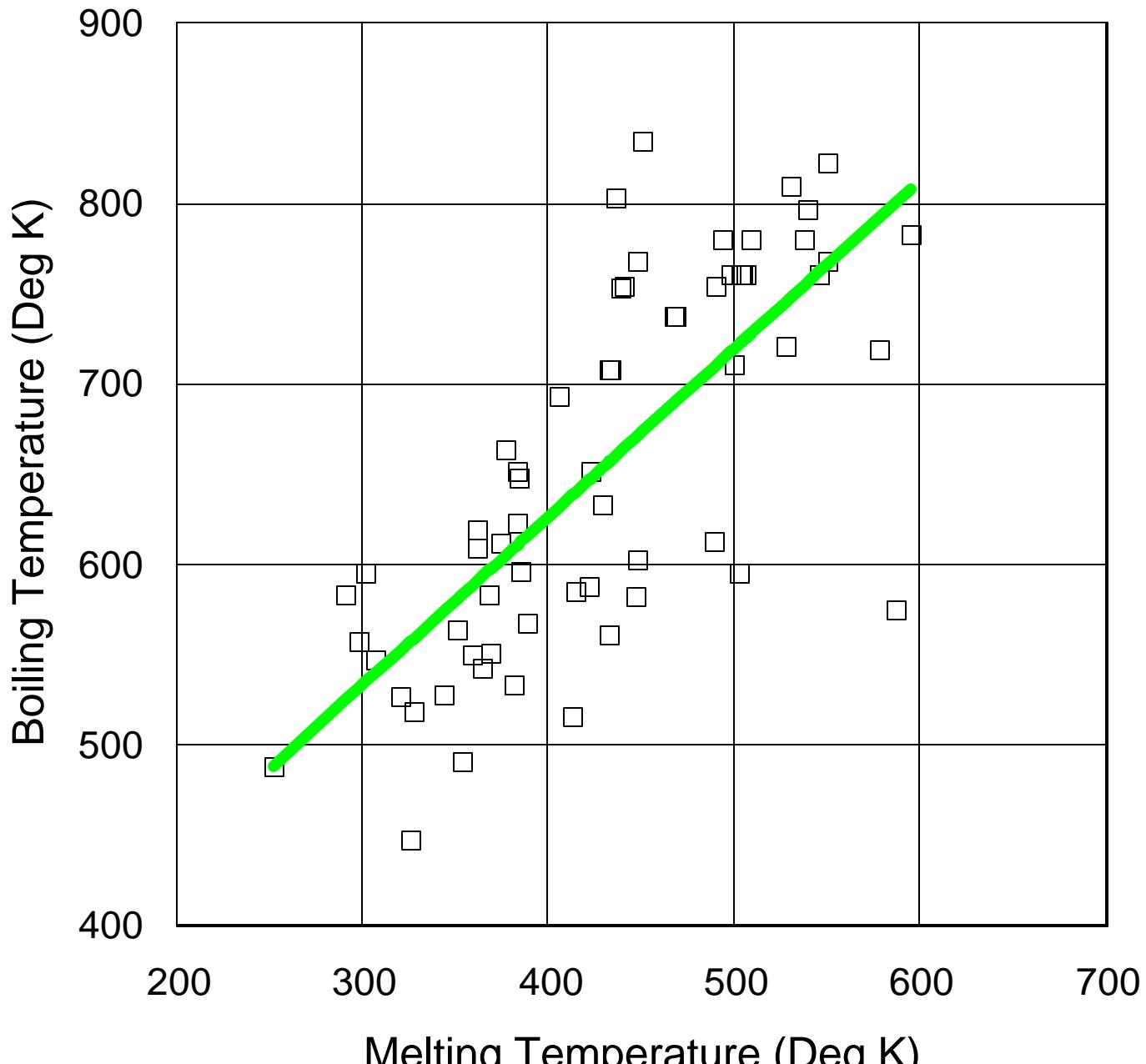
Ref 97 = National Library of Medicine, Hazardous Substances Data Base (HSDB) [various searches: Dec 96, Jan 97]

TYPE	CHEMICAL IDENTITY DATA			Water Solubility							ratio of dinitro to parent		
	compound	cas #	molecular weight	solubility	units	standard units	notes on conversion to std units	temp	temp units	ref	notes	ratio of dinitro to parent	avg for chemical group
parent	Benzene	71-43-2	78.11	0.18	g/100 g wat	1800		25	deg C	97			
+ 1 nitro	Benzene, nitro-	98-95-3	123.11	1780	ppm	1780	assume ppm by weight	not given		97			
+2 nitro's	benzene, 1,2-dinitro-	528-29-0	168.11	*****	g/ml	152		"cold water"		97		0.08	0.11
+2 nitro's	benzene, 1,3-dinitro-	99-65-0	168.11	2.2	mol/m3	370		not given		97		0.21	0.11
+2 nitro's	benzene, 1,4-dinitro-	100-25-4	168.11	0.00008	g/ml	80		not given		97		0.04	0.11
parent	Naphthalene	91-20-3	128.17	30	mg/lit	30		not given		97			
+ 1 nitro	naphthalene, 1-nitro-	86-57-7	173.17	18	mg/lit	18		not given		97	estimated		
parent	Cresol	1319-77-3		50	parts water	20000	assume by weight	not given					
+ 1 nitro													
+2 nitro's	Cresol, 4,6-dinitro-o	534-52-1	198.13	130	mg/lit	130		15	deg C	97		0.0065	0.011
+2 nitro's	Cresol, 2,6-dinitro-p	609-93-8	198.13	290	mg/lit	290		15	deg C	97		0.0145	0.011
parent	Phenol	108-95-2	**	*****	g/ml	66667		not given					
+ 1 nitro													
+2 nitro's	Phenol, 2,3-dinitro		184.1	2200	mg/lit	2200		35.5	deg C	97		0.033	0.011
+2 nitro's	Phenol, 2,4-dinitro		184.1	790	mg/lit	790		35.5	deg C	97		0.012	0.011
+2 nitro's	Phenol, 2,5-dinitro		184.1	680	mg/lit	680		35.5	deg C	97		0.010	0.011
+2 nitro's	Phenol, 2,6-dinitro		184.1	420	mg/lit	420		35.5	deg C	97		0.006	0.011
+2 nitro's	Phenol, 3,4-dinitro		184.1	230	mg/lit	230		35.5	deg C	97		0.003	0.011
+2 nitro's	Phenol, 3,5-dinitro		184.1	160	mg/lit	160		35.5	deg C	97		0.002	0.011
parent	Pyrene	129-00-0		0.135	mg/lit	0.135		25	deg C	97			
+ 1 nitro													
+2 nitro's													

#### **Appendix B.4.**

**Methodology Used to Estimate Boiling Temperature  
When No Data Were Available**  
**(based on Regression Between Melting Temperature  
and Boiling Temperature for Other Compounds)**

## Boiling Temperature vs. Melting Temperature For BVES Compounds with Available Data



Line is Best-Fit Linear Regression

IS THERE A CRUDE RELATIONSHIP BETWEEN MELTING and BOILING TEMP?; Following Table has Available Data for BVES Compounds sorted in Ascending Melting Point Order				
common chemical name	cas # (1)	PHYSICAL STATE		
		physical state		reference
		calc'd (probably molecular at room	temperature)	
hexachloro-1,3-butadiene	000087-68-3	260.7	liquid	considering Tm
4-bromophenyl phenyl ether	000101-55-3	249.1	varies; melt temp ~ 18 deg C	considering Tm
3-PCB	002051-61-8	188.7	varies	Tm near room temp
3,3'-PCB	002050-67-1	223.1	varies	Tm near room temp
2-PCB	002051-60-7	188.7	varies	Tm near room temp
1,2,3,4-tetrachlorobenzene	000634-66-2	215.9	solid	considering Tm
1,4-dichlorobenzene	000106-46-7	147.0	solid	considering Tm
1,2,3,5-tetrachlorobenzene	000634-90-2	215.9	solid	considering Tm
biphenyl	000092-54-2	154.2	solid	considering Tm
4-PCB	002051-62-9	188.7	solid	considering Tm
naphthalene	000091-20-3	106.2	solid	considering Tm
pentachlorobenzene	000608-93-5	250.3	solid	considering Tm
methoxychlor	000072-43-5	345.6	solid	considering Tm
p,p'-DDE	000072-55-9	318.0	crystalline solid	60; also consistent with Tm
acenaphthylene	000208-96-8	152.2	solid	considering Tm
heptachlor	000076-44-8	373.3	crystalline solid	53; also consistent with Tm
acenaphthene	000083-32-9	154.2	solid	considering Tm
phenanthrene	000085-01-8	178.2	solid	considering Tm
aldrin	000309-00-2	364.9	crystalline solid	47; also consistent with Tm
p,p'-DDT	000050-29-3	354.5	crystalline solid	59; also consistent with Tm
4'-methylene bis(2-chloroaniline)	000101-14-4	267.2	solid	considering Tm
p,p'-DDD	000072-54-8	320.0	crystalline solid	60; also consistent with Tm
fluoranthene	000206-44-0	202.3	solid	considering Tm
gamma-hexachlorocyclohexane	000058-89-9	290.8	crystalline solid	33; also consistent with Tm
fluorene	000086-73-7	166.2	solid	considering Tm
3,3'-dichlorobenzidene	000091-94-1	253.1	solid	considering Tm
1,2,4,5-tetrachlorobenzene	000095-94-3	215.9	solid	considering Tm
delta-hexachlorocyclohexane	000319-86-8	290.8	fine plates	29; also consistent with Tm
4,4'-PCB	002050-68-2	223.1	solid	considering Tm
octachlorostyrene	029082-74-4	379.7		
pyrene	000129-00-0	202.3	solid	considering Tm
alpha-hexachlorocyclohexane	000319-84-6	290.8	crystalline solid	32; also consistent with Tm
benz [ a ] anthracene	000056-55-3	228.3	solid	considering Tm
heptachlor epoxide	001024-57-3	389.3	crystalline solid	53; ref 52 says that its liqui
indeno [ 1,2,3-c,d ] pyrene	000193-39-5	276.3	solid	considering Tm
benzo [ j ] fluoranthene	000205-82-2	252.3	solid	considering Tm
benzo [ b ] fluoranthene	000205-99-2	252.3	solid	considering Tm
pentachlorophenol	000087-86-5	266.3	flakes or crystalline solid	42; also consistent with Tm
benzo [ a ] pyrene	000050-32-8	252.3	solid	considering Tm

IS THERE A CRUDE RELATIONSHIP BETWEEN MELTING and BOILING TEMP?; Following Table has Available Data for BVES Compounds sorted in Ascending Melting Point Order				
NAME		PHYSICAL STATE		
common chemical name	cas # (1)	calc'd molecular weight	physical state (probably at room temperature)	reference
dieldrin	000060-57-1	380.9	crystalline solid	47; also consistent with Tm
benzo [ e ] pyrene	000192-97-2	252.3	solid	considering Tm
1,2,3,7,8-PeCDD	040321-76-4	356.4	solid	considering Tm
1,2,3,7,8-PeCDF	057117-41-6	340.4	solid	considering Tm
2,3,4,7,8-PeCDF	057117-31-4	340.4	solid	considering Tm
anthracene	000120-12-7	178.2	solid	considering Tm
benzo [ k ] fluoranthene	000207-08-9	252.3	solid	considering Tm
1,2,3,4,7,8,9-HxCDF	055673-89-7	409.3	solid	considering Tm
1,2,3,4,7,8-HxCDF	070648-26-9	374.8	solid	considering Tm
2,3,7,8-TCDF	051207-31-9	306.0	solid	considering Tm
hexachlorobenzene	000118-74-1	284.8	solid	considering Tm
1,2,3,6,7,8-HxCDF	057117-44-9	374.8	solid	considering Tm
1,2,3,4,6,7,8-HpCDF	067562-39-4	409.3	solid	considering Tm
2,3,4,6,7,8-HxCDF	060851-34-5	374.8	solid	considering Tm
1,2,3,7,8,9-HxCDF	072918-21-9	374.8	solid	considering Tm
chrysene	000218-01-9	228.3	solid	considering Tm
OCDF	039001-02-0	443.7	solid	considering Tm
1,2,3,4,6,7,8-HpCDD	035822-46-9	425.3	solid	considering Tm
dibenzo [ a,h ] anthracene	000053-70-1	278.4	solid	considering Tm
1,2,3,4,7,8-HxCDD	039227-28-6	390.8	solid	considering Tm
1,2,3,6,7,8-HxCDD	057653-85-7	390.8	solid	considering Tm
1,2,3,7,8,9-HxCDD	019408-74-3	390.8	solid	considering Tm
perylene	000198-55-0	252.3	solid	considering Tm
benzo [ g,h,i ] perylene	000191-24-2	268.4	solid	considering Tm
2,3,7,8-TCDD	001746-01-6	322.0	solid	considering Tm
beta-hexachlorocyclohexane	000319-85-7	290.8	crystalline solid	33; also consistent with Tm
OCDD	003268-87-9	459.7	solid	considering Tm
mirex				
toxaphene			waxy solid	consistent with Tm
endrin			crystalline solid	consistent with Tm
monomethyl mercury chloride			solid	consistent with Tm
2,7-dinitropyrene	117929-15-4	292.3	probably solid	considering Tm of 1,6 DNP
dinitropyrenes (mixed)	078432-19-6	292.3	probably solid	considering Tm of 1,6 DNP
1,3-dinitropyrene	075321-20-9	292.3	probably solid	considering Tm of 1,6 DNP
1,6-dinitropyrene	042397-64-8	292.3	probably solid	considering Tm of 1,6 DNP
1,8-dinitropyrene	042397-65-9	292.3	probably solid	considering Tm of 1,6 DNP

IS THERE A CRUDE RELATIONSHIP BETWEEN MELTING and BOILING TEMP?; Following Table has Available Data for BVES Compounds sorted in Ascending Melting Point Order							
NAME	MELTING POINT						
	for V/P						
	melting point	data					
common chemical name	cas # (1)	range	average	units	ref	deg K	notes
hexachloro-1,3-butadiene	000087-68-3		-21	deg C	7	252	
4-bromophenyl phenyl ether	000101-55-3		18	deg C	7	291	
3-PCB	002051-61-8		25	deg C	5	298	
3,3'-PCB	002050-67-1		29	deg C	5	302	
2-PCB	002051-60-7		34	deg C	5	307	
1,2,3,4-tetrachlorobenzene	000634-66-2		48	deg C	5	321	similar in Aldrich catalog
1,4-dichlorobenzene	000106-46-7		53	deg C	5	326	similar in Aldrich catalog
1,2,3,5-tetrachlorobenzene	000634-90-2		55	deg C	5	328	
biphenyl	000092-54-2		71	deg C	5	344	
4-PCB	002051-62-9		78	deg C	5	351	
naphthalene	000091-20-3		81	deg C	6	354	
pentachlorobenzene	000608-93-5		86	deg C	5	359	similar in Aldrich catalog
methoxychlor	000072-43-5		89	deg C	24; 85	362	
p,p'-DDE	000072-55-9	88-90	89	deg C?	aldrich cata	362	same in ref 61 and SRC data set
acenaphthylene	000208-96-8		92	deg C	6	365	
heptachlor	000076-44-8	95-96	96	deg C	25	369	same in ref 85
acenaphthene	000083-32-9		96	deg C	6	369	
phenanthrene	000085-01-8		101	deg C	6	374	
aldrin	000309-00-2		104	deg C	25	377	
p,p'-DDT	000050-29-3	107-110	109	deg C?	aldrich cata	382	same in ref 61
4'-methylene bis(2-chloroaniline)	000101-14-4		110	deg C	15	383	
p,p'-DDD	000072-54-8	109-111	110	deg C?	aldrich cata	383	same in ref 61
fluoranthene	000206-44-0		111	deg C	6	384	
gamma-hexachlorocyclohexane	000058-89-9		113	deg C	29, 30	386	
fluorene	000086-73-7		116	deg C	6	389	
3,3'-dichlorobenzidine	000091-94-1	132-133	133	deg C	Howard, Vg	406	same in ref 8
1,2,4,5-tetrachlorobenzene	000095-94-3		140	deg C	5	413	similar in Aldrich catalog
delta-hexachlorocyclohexane	000319-86-8		142	deg C	29	415	
4,4'-PCB	002050-68-2		149	deg C	5	422	
octachlorostyrene	029082-74-4		150	deg C	89	423	estimated using linear regression; not in
pyrene	000129-00-0		156	deg C	6	429	
alpha-hexachlorocyclohexane	000319-84-6		160	deg C	29	433	
benz [ a ] anthracene	000056-55-3		160	deg C	6	433	
heptachlor epoxide	001024-57-3	160-161.5	161	deg C	25	434	same in ref 85
indeno [ 1,2,3-c,d ] pyrene	000193-39-5		164	deg C	9	437	
benzo [ j ] fluoranthene	000205-82-2		166	deg C	6	439	
benzo [ b ] fluoranthene	000205-99-2		168	deg C	6	441	
pentachlorophenol	000087-86-5		174	deg C	8	447	
benzo [ a ] pyrene	000050-32-8		175	deg C	6	448	

IS THERE A CRUDE RELATIONSHIP BETWEEN MELTING and BOILING TEMP?; Following Table has Available Data for BVES Compounds sorted in Ascending Melting Point Order						
NAME	MELTING POINT for V/P					
	melting point	melting point	melting point	melting point	melting point	data
common chemical name	cas # (1)	range	average	units	ref	deg K
						notes
dieldrin	000060-57-1	175-176	176	deg C	25	449
benzo [ e ] pyrene	000192-97-2		178	deg C	6	451
1,2,3,7,8-PeCDD	040321-76-4		195	deg C	6	468
1,2,3,7,8-PeCDF	057117-41-6		196	deg C	6	469
2,3,4,7,8-PeCDF	057117-31-4		196	deg C	6	469
anthracene	000120-12-7		216	deg C	6	489
benzo [ k ] fluoranthene	000207-08-9		217	deg C	6	490
1,2,3,4,7,8,9-HxCDF	055673-89-7		221	deg C	6	494
1,2,3,4,7,8-HxCDF	070648-26-9		226	deg C	6	499
2,3,7,8-TCDF	051207-31-9		227	deg C	6	500
hexachlorobenzene	000118-74-1		230	deg C	5	503
1,2,3,6,7,8-HxCDF	057117-44-9		232	deg C	6	505
1,2,3,4,6,7,8-HxCDF	067562-39-4		236	deg C	6	509
2,3,4,6,7,8-HxCDF	060851-34-5		231	deg C	6	504
1,2,3,7,8,9-HxCDF	072918-21-9		234	deg C	6	507
chrysene	000218-01-9		255	deg C	6	528
OCDF	039001-02-0		258	deg C	6	531
1,2,3,4,6,7,8-HxCDD	035822-46-9		265	deg C	6	538
dibenz [a,h] anthracene	000053-70-1		267	deg C	6	540
1,2,3,4,7,8-HxCDD	039227-28-6		273	deg C	6	546
1,2,3,6,7,8-HxCDD	057653-85-7		273	deg C	6	546
1,2,3,7,8,9-HxCDD	019408-74-3		273	deg C	6	546
perylene	000198-55-0		277	deg C	6	550
benzo [ g,h,i ] perylene	000191-24-2		277	deg C	6	550
2,3,7,8-TCDD	001746-01-6		305	deg C	6	578
beta-hexachlorocyclohexane	000319-85-7		315	deg C	29	588
OCDD	003268-87-9		322	deg C	6	595
mirex						758
toxaphene		65-90	77.5	deg C	25	351
endrin		226-230	228.0	deg C	25	501
monomethyl mercury chloride			170.0	deg C	95	443
2,7-dinitropyrene	117929-15-4				479	crude: pyrene+50 C
dinitropyrenes (mixed)	078432-19-6				479	crude: pyrene+50 C
1,3-dinitropyrene	075321-20-9				479	crude: pyrene+50 C
1,6-dinitropyrene	042397-64-8	> 300		deg C	aldrich cata	479
1,8-dinitropyrene	042397-65-9					479

IS THERE A CRUDE RELATIONSHIP BETWEEN MELTING and BOILING TEMP?; Following Table has Available Data for BVES Compounds sorted in Ascending Melting Point Order												
NAME		BOILING POINT										
		for V/P			boiling			T boil				
		boiling	boiling	boiling	boiling	boiling	point	estimated	percent			
		point	point	point	point	point	data	using	error			
common chemical name	cas # (1)	range	average	units	ref	deg K	notes	regression	in			
								deg K	estimate			
hexachloro-1,3-butadiene	000087-68-3	215	deg C	19	488			489	0%			
4-bromophenyl phenyl ether	000101-55-3	310	deg C	7	583			525	-10%			
3-PCB	002051-61-8	284	deg C	5	557			532	-5%			
3,3'-PCB	002050-67-1	322	deg C	5	595			535	-10%			
2-PCB	002051-60-7	274	deg C	5	547			540	-1%			
1,2,3,4-tetrachlorobenzene	000634-66-2	254	deg C	5	527	similar in Aldrich catalog		552	5%			
1,4-dichlorobenzene	000106-46-7	175	deg C	5	448			558	25%			
1,2,3,5-tetrachlorobenzene	000634-90-2	246	deg C	5	519			559	8%			
biphenyl	000092-54-2	255	deg C	5	528			574	9%			
4-PCB	002051-62-9	291	deg C	5	564			581	3%			
naphthalene	000091-20-3	218	deg C	6	491			583	19%			
pentachlorobenzene	000608-93-5	277	deg C	5	550	similar in Aldrich catalog		588	7%			
methoxychlor	000072-43-5	346	deg C	85	619	one ref says that it decomposes when heated, so no data.		591	-5%			
p,p'-DDE	000072-55-9	336	deg C	85	609			591	-3%			
acenaphthylene	000208-96-8	265-275	270	deg C	6	543		594	9%			
heptachlor	000076-44-8	310	deg C	85	583			597	2%			
acenaphthene	000083-32-9	278	deg C	6	551			598	9%			
phenanthrene	000085-01-8	339	deg C	6	612			602	-2%			
aldrin	000309-00-2	664	deg K	87	664	estimated using Clausius Clapyron equation		605	-9%			
p,p'-DDT	000050-29-3	260	deg C	60	533	not given in ref 85		609	14%			
4'-methylene bis(2-chloroaniline)	000101-14-4	379	deg C	83	652			611	-6%			
p,p'-DDD	000072-54-8	350	deg C	85	623			611	-2%			
fluoranthene	000206-44-0	375	deg C	6	648			612	-6%			
gamma-hexachlorocyclohexane	000058-89-9	323	deg C	31	597			613	3%			
fluorene	000086-73-7	295	deg C	6	568			616	8%			
3,3'-dichlorobenzidine	000091-94-1	420	deg C	18	693			632	-9%			
1,2,4,5-tetrachlorobenzene	000095-94-3	243	deg C	5	516	similar in Aldrich catalog		639	24%			
delta-hexachlorocyclohexane	000319-86-8	312	deg C	29	586	estm based on 60 deg C @ 0.36 mm Hg		640	9%			
4,4'-PCB	002050-68-2	315	deg C	5	588			647	10%			
octachlorostyrene	029082-74-4	379	deg C	89	652	estimated using linear regression; not in SRC database		648	-1%			
pyrene	000129-00-0	360	deg C	6	633			653	3%			
alpha-hexachlorocyclohexane	000319-84-6	288	deg C	31	561			657	17%			
benz [ a ] anthracene	000056-55-3	435	deg C	6	708			657	-7%			
heptachlor epoxide	001024-57-3	no data			708	No data available; use value for heptachlor for now		658	-7%			
indeno [ 1,2,3-c,d ] pyrene	000193-39-5	530	deg C	11	803			660	-18%			
benzo [ j ] fluoranthene	000205-82-2	480	deg C	6	753			663	-12%			
benzo [ b ] fluoranthene	000205-99-2	481	deg C	6	754			665	-12%			
pentachlorophenol	000087-86-5	310	deg C	25	583	decomposes		670	15%			
benzo [ a ] pyrene	000050-32-8	495	deg C	6	768			671	-13%			

IS THERE A CRUDE RELATIONSHIP		BETWEEN MELTING and BOILING TEMP?; Following Table has Available Data for BVES Compounds sorted in Ascending Melting Point Order									
		NAME							BOILING POINT		
		for V/P							T boil		
		boiling	boiling	boiling	boiling	boiling	point	boiling	estimated	percent	
		point	point	point	point	point	point	point	using	error	
		common chemical name	cas # (1)	range	average	units	ref	deg K	notes	regression	in
								deg K		deg K	estimate
dieldrin	000060-57-1		330	deg C	48		603	estim'd?; same data given in SRC data set	672	11%	
benzo [ e ] pyrene	000192-97-2		561	deg C	79		835	Estimated using calculation; value not given in Ref 6; 310-3	674	-19%	
1,2,3,7,8-PeCDD	040321-76-4		465	deg C	6		738	using value for 12347 PeCDD	690	-7%	
1,2,3,7,8-PeCDF	057117-41-6		465	deg C	6		738	using value for 23478 PeCDF	691	-6%	
2,3,4,7,8-PeCDF	057117-31-4		465	deg C	6		738		691	-6%	
anthracene	000120-12-7		340	deg C	6		613		709	16%	
benzo [ k ] fluoranthene	000207-08-9		481	deg C	6		754		710	-6%	
1,2,3,4,7,8,9-HxCDF	055673-89-7		507	deg C	6		780		714	-9%	
1,2,3,4,7,8-HxCDF	070648-26-9		488	deg C	6		761		718	-6%	
2,3,7,8-TCDF	051207-31-9		438	deg C	6		711		720	1%	
hexachlorobenzene	000118-74-1		322	deg C	5		595	similar in Aldrich catalog	722	21%	
1,2,3,6,7,8-HxCDF	057117-44-9		488	deg C	6		761		724	-5%	
1,2,3,4,6,7,8-HxCDF	067562-39-4		507	deg C	6		780		728	-7%	
2,3,4,6,7,8-HxCDF	060851-34-5		488	deg C	6		761	using avg of values for 123478 HxCDF and 123678 HxCDF	723	-5%	
1,2,3,7,8,9-HxCDF	072918-21-9		488	deg C	6		761	using avg of values for 123478 HxCDF and 123678 HxCDF	726	-5%	
chrysene	000218-01-9		448	deg C	6		721		746	3%	
OCDF	039001-02-0		537	deg C	6		810		748	-8%	
1,2,3,4,6,7,8-HxCDD	035822-46-9		507	deg C	6		780		755	-3%	
dibenz [ a,h ] anthracene	000053-70-1		524	deg C	6		797		757	-5%	
1,2,3,4,7,8-HxCDD	039227-28-6		488	deg C	6		761		762	0%	
1,2,3,6,7,8-HxCDD	057653-85-7		488	deg C	6		761	using value for 123478 HxCDD	762	0%	
1,2,3,7,8,9-HxCDD	019408-74-3		488	deg C	6		761	using value for 123478 HxCDD	762	0%	
perylene	000198-55-0		495	deg C	6		768		766	-0%	
benzo [ g,h,i ] perylene	000191-24-2		550	deg C	11		823		766	-7%	
2,3,7,8-TCDD	001746-01-6		447	deg C	6		720		792	10%	
beta-hexachlorocyclohexane	000319-85-7		302	deg C	29		575	estm based on 60 deg C @ 0.5 mm Hg	801	39%	
OCDD	003268-87-9		510	deg C	6		783		808	3%	
mirex									960		
toxaphene									580		
endrin									720		
monomethyl mercury chloride									666		
2,7-dinitropyrene	117929-15-4						683	crude: pyrene + 50 C	700		
dinitropyrenes (mixed)	078432-19-6						683	crude: pyrene + 50 C	700		
1,3-dinitropyrene	075321-20-9						683	crude: pyrene + 50 C	700		
1,6-dinitropyrene	042397-64-8						683	crude: pyrene + 50 C	700		
1,8-dinitropyrene	042397-65-9						683	crude: pyrene + 50 C	700		

IS THERE A CRUDE RELATIONSHIP  
BETWEEN MELTING and BOILING  
TEMP?; Following Table has Available  
Data for BVES Compounds  
sorted in Ascending Melting  
Point Order

NAME	common chemical name	cas # (1)	BOILING POINT						T boil estimated using regression deg K	percent error in estimate	
			boiling point range	boiling point average	boiling point units	boiling point ref	boiling point deg K	boiling point data			
dieldrin		000060-57-1		330 deg C	48	603	estim'd?; same data given in SRC data set			672 11%	
benzo [ e ] pyrene		000192-97-2		561 deg C	79	835	Estimated using calculation; value not given in Ref 6; 310-3			674 -19%	
1,2,3,7,8-PeCDD		040321-76-4		465 deg C	6	738	using value for 12347 PeCDD			690 -7%	
1,2,3,7,8-PeCDF		057117-41-6		465 deg C	6	738	using value for 23478 PeCDF			691 -6%	
2,3,4,7,8-PeCDF		057117-31-4		465 deg C	6	738				691 -6%	
anthracene		000120-12-7		340 deg C	6	613				709 16%	
benzo [ k ] fluoranthene		000207-08-9		481 deg C	6	754				710 -6%	
1,2,3,4,7,8,9-HxCDF		055673-89-7		507 deg C	6	780				714 -9%	
1,2,3,4,7,8-HxCDF		070648-26-9		488 deg C	6	761				718 -6%	
2,3,7,8-TCDF		051207-31-9		438 deg C	6	711				720 1%	
hexachlorobenzene		000118-74-1		322 deg C	5	595	similar in Aldrich catalog			722 21%	
1,2,3,6,7,8-HxCDF		057117-44-9		488 deg C	6	761				724 -5%	
1,2,3,4,6,7,8-HxCDF		067562-39-4		507 deg C	6	780				728 -7%	
2,3,4,6,7,8-HxCDF		060851-34-5		488 deg C	6	761	using avg of values for 123478 HxCDF and 123678 HxCDF			723 -5%	
1,2,3,7,8,9-HxCDF		072918-21-9		488 deg C	6	761	using avg of values for 123478 HxCDF and 123678 HxCDF			726 -5%	
chrysene		000218-01-9		448 deg C	6	721				746 3%	
OCDF		039001-02-0		537 deg C	6	810				748 -8%	
1,2,3,4,6,7,8-HxCDD		035822-46-9		507 deg C	6	780				755 -3%	
dibenz [ a,h ] anthracene		000053-70-1		524 deg C	6	797				757 -5%	
1,2,3,4,7,8-HxCDD		039227-28-6		488 deg C	6	761				762 0%	
1,2,3,6,7,8-HxCDD		057653-85-7		488 deg C	6	761	using value for 123478 HxCDD			762 0%	
1,2,3,7,8,9-HxCDD		019408-74-3		488 deg C	6	761	using value for 123478 HxCDD			762 0%	
perylene		000198-55-0		495 deg C	6	768				766 -0%	
benzo [ g,h,i ] perylene		000191-24-2		550 deg C	11	823				766 -7%	
2,3,7,8-TCDD		001746-01-6		447 deg C	6	720				792 10%	
beta-hexachlorocyclohexane		000319-85-7		302 deg C	29	575	estm based on 60 deg C @ 0.5 mm Hg			801 39%	
OCDD		003268-87-9		510 deg C	6	783				808 3%	
mirrex										960	
toxaphene										580	
endrin										720	
monomethyl mercury chloride										666	
2,7-dinitropyrene		117929-15-4				683	crude: pyrene + 50 C			700	
dinitropyrenes (mixed)		078432-19-6				683	crude: pyrene + 50 C			700	
1,3-dinitropyrene		075321-20-9				683	crude: pyrene + 50 C			700	
1,6-dinitropyrene		042397-64-8				683	crude: pyrene + 50 C			700	
1,8-dinitropyrene		042397-65-9				683	crude: pyrene + 50 C			700	

## **Appendix C.**

# **Vapor/Particle Partitioning**

- C.1. Vapor/Particle Partitioning Theory**
- C.2. Results of Vapor/Particle Partitioning Estimates**
- C.3. Comparison of Vapor/Particle Partitioning Estimates with Examples of Vapor/Particle Partitioning Measurements from the Literature**
- C.4. Vapor-Particle Partitioning of PAH's: Detailed Comparison of Theoretical Estimates with Recent Experimental Data**

## Appendix C.1.

### Vapor/Particle Partitioning Theory

In the atmosphere, pollutants can exist, generally, in the vapor phase or associated with particles, i.e., the aerosol phase. For semivolatile compounds there can be significant fractions associated with either phase. This phenomenon is of crucial importance in determining the fate of semivolatile compounds in the atmosphere, because each of the deposition and destruction mechanisms depend a great deal on the physical form of the pollutant. The vapor/particle partitioning phenomenon was first introduced by Junge (1977), and has been extended and reviewed by many, including the following: Eisenreich et al 1981; Bidleman et al 1986; Bidleman and Foreman, 1987; Foreman and Bidleman, 1987; Bidleman 1988; Pankow 1987, 1988, 1991; Pankow and Bidleman, 1991, 1992; and Johnson et al, 1990. The phenomenon as it relates to atmospheric PCDD/PCDF has been recently measured (Nakano et al, 1990) and summarized (USEPA 1994A).

In essence, the theory of vapor-particle partitioning postulates that for any species in the atmosphere, there is an equilibrium between vapor phase and the particle phase that depends primarily on the physical-chemical properties of the species of interest, the nature of the atmospheric aerosol, and the temperature. As proposed by Junge (1977), the vapor-particle partitioning of exchangeable material can be estimated from the following equation:

$$\Phi = c S_t / (p(T) + cS_t)$$

where

$\Phi$  = the fraction of the total mass of the species absorbed to the particle phase (dimensionless)

$S_t$  = the total surface area of particles, per unit volume of air ( $\text{cm}^2/\text{cm}^3$ )

$p(T)$  = the saturation vapor pressure of the species of interest (atm), at the ambient temperature ( $T$ )

$c$  = an empirical constant, estimated by Junge to be approximately  $1.7 \times 10^{-4}$  atm-cm

The most thermodynamically stable form of many semivolatile species at ambient temperatures is typically a solid, but, Bidleman (1988) has argued that it is the "non-equilibrium" or subcooled liquid phase which controls the dynamic equilibrium partitioning of such compounds between the vapor phase and the atmospheric aerosol. Thus, the subcooled liquid vapor pressure at the ambient temperature should be used in the above equation. This vapor pressure can be approximately estimated from the following equation:

$$\ln(P/P_s) = \Delta S_f (T_m - T) / RT$$

where

$P_l$  = subcooled liquid vapor pressure (atm) at temp.  $T$

$P_s$  = solid vapor pressure (atm) at temperature  $T$

$\Delta S_f$  = entropy of fusion ( $\text{atm m}^3/\text{mole deg K}$ )  
(approximately equal to 6.79 R)

$T_m$  = melting temperature of the solid compound (deg K)

$T$  = ambient temperature (deg K)

$R$  = the gas constant ( $\text{atm m}^3/\text{mole deg K}$ )

Mackay et al (1986) have suggested that the solid vapor pressure at the temperature of interest

can be estimated from the reported solid vapor pressure at a standard temperature with the Clausius-Clapeyron equation using the enthalpy of vaporization, according to the following equation:

$$\ln(P_s^s_1 / P_s^s_2) = (\Delta H / R) (1/T_2 - 1/T_1)$$

where

$P_s^s_1$  = solid vapor pressure (atm) at temperature  $T_1$

$P_s^s_2$  = solid vapor pressure (atm) at temperature  $T_2$

$\Delta H$  = enthalpy of vaporization (J/mole)

Note: according to Trouton's Rule,  $\Delta H$  can be approximately estimated by the following relation:  $\Delta H / T_{boil} = 84 \text{ J}/(\text{mol degK})$  (Mackay et al 1986).

$R$  = gas constant (J/mole degK [=] (atm  $\text{m}^3/\text{mole deg K}$ )

$T_2$  = temperature 1 (deg K)

$T_1$  = temperature 2 (deg K)

Thus, the vapor particle partitioning for a given compound in the atmosphere can be estimated from the first of the above two equations, with  $P_s^s$  from the second equation used for  $P(T)$ . From the foregoing, it is seen that the only species-specific physical-chemical property data required to make a vapor/particle partitioning estimate according to the above simplified approach are the species' solid vapor pressure at one temperature, and the species' boiling and melting temperatures.

It is typically assumed that semivolatile compounds in the atmosphere are "fully exchangeable", i.e., that the compound can move freely between the vapor and particle phases, depending on the dictates of thermodynamics. To the extent that a portion of the material was "locked-up" within particles and was not available for exchange, this assumption would be in error.

There is some experimental evidence that suggests that many semivolatile compounds are indeed fully exchangeable in the atmosphere. For example, Eitzer and Hites (1989a and 1989c) measured vapor- and particulate-phase PCDD/F in the atmosphere of Bloomington, IN and found that while there was no temperature-related effect on the total concentration of PCDD/F in the atmosphere, the proportions in the two phases were dependent on the ambient temperature at the time of the measurement. Further, in agreement with V/P theory, it was found that the V/P partitioning of each of the congeners was dependent on each congener's subcooled liquid vapor pressure (Eitzer and Hites, 1989a).<sup>9</sup>

Some compounds, such as HCB, are predicted and found to exist predominantly in the vapor phase, and the issue of exchangeability is moot.

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<sup>9</sup> Koester and Hites (1992) measured wet and dry deposition of atmospheric PCDD/F, and found that dry deposition was inversely related to ambient temperature. These authors assumed that vapor-phase dry deposition was negligible and that only particle-phase dry deposition was significant. With this assumption, their results are consistent with the hypothesis that the proportion of vapor-phase and particle-phase PCDD/F changes with ambient temperature. On the other hand, if their assumption of vapor-phase deposition being insignificant is not valid, then their finding is not relevant to the vapor/particle exchangeability issue.

Vapor/particle partitioning of PAH's is found to vary with ambient temperature (e.g., Yamasaki et al., 1982) suggesting that most or all of PAH's in the atmosphere are exchangeable. Kamens et al. (1995) have suggested that the equilibration time for atmospheric PAH's may be relatively long (on the order of hours) because of mass transfer resistance within organic layers on atmospheric particles.

### Aerosol Characteristics

As described above in the formulation of the vapor/particle partitioning equations, the aerosol surface area plays a role in determining the vapor/particle partitioning behavior of a compound in the atmosphere. Bidleman (1988), citing a study by Whitby (1978), summarizes data on the total aerosol surface area found in measurements. These "typical values" are summarized in the table below. In reality, the characteristics of the atmospheric aerosol vary from point to point in the atmosphere, and at any given point, changes with time.

<b>Table _____. Typical Aerosol Surface Areas per Unit Volume</b> [from Whitby (1978)]	
<b>Type of Atmospheric Location</b>	<b>Typical Aerosol Surface Area (cm<sup>2</sup> surface area / cm<sup>3</sup> air)</b>
Clean Continental Background	$4.2 \times 10^{-7}$
Average Background	$1.5 \times 10^{-6}$
Background + Local Sources	$3.5 \times 10^{-6}$
Urban	$1.1 \times 10^{-5}$

### Uncertainties

There are many uncertainties associated with vapor/particle partitioning theory and measurements.

For example, the vapor pressure of many compounds is relatively uncertain, with reported values often differing by more than an order of magnitude. Moreover, the estimation of subcooled liquid vapor pressures from solid phase values introduces additional uncertainties. In addition, the surface area of the atmospheric aerosol can vary widely. Thus, even if the above theory "perfectly" described the vapor/particle partitioning phenomenon, there would be large uncertainties related to uncertainties in vapor pressure and aerosol surface area. Possible deviations from the above theory due to the effects of relative humidity, non-exchangeable material and intra-particle mass-transfer phenomena (possibly important for PAH's, for example) also indicate that the estimates made here are somewhat uncertain. Compounds that are predicted in this analysis to exist *overwhelmingly* in either the vapor or particle phase probably exist in the predicted phase, but, it is acknowledged that for *intermediate* compounds, the estimates for the relative proportion of vapor and particle fractions is relatively uncertain.

Thibodeaux et al (1991) have extended the theory of vapor/particle partitioning of semivolatile organic compounds (SOC) to include the effect of the competition of water vapor for adsorption sites on an atmospheric particle before deliquescence. The effect of moisture was shown to reduce the fraction of the SOC that is predicted to be adsorbed to atmospheric particles.

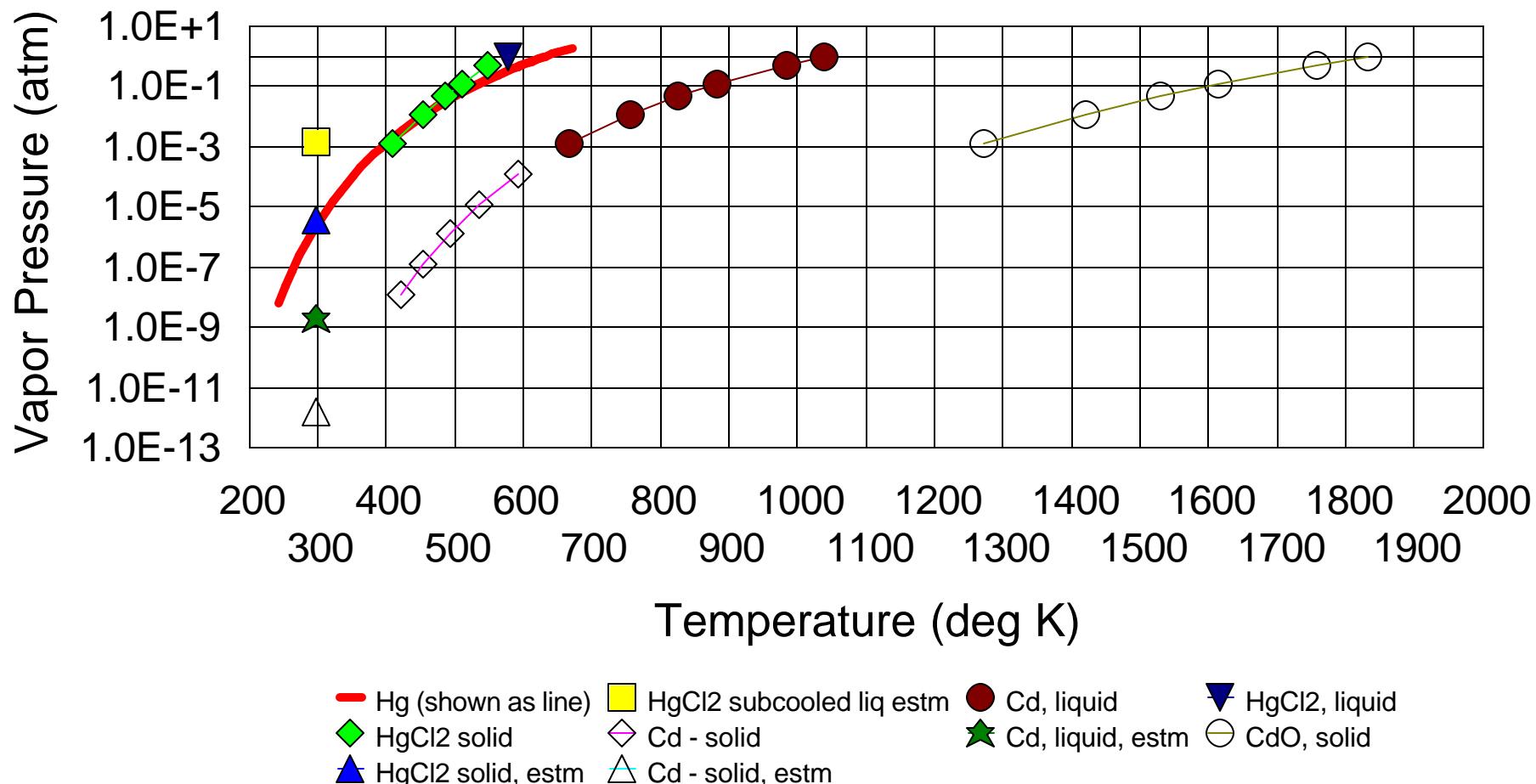
Rounds and Pankow (1990) considered the mass transfer aspects of vapor/particle partitioning and concluded that vapor/particle equilibrium would be achieved in several hours or less, depending on the compound.

More recently, Rounds et al. (1993) attempted to measure the vapor/particle partitioning of selected PAH's and other compounds in a laboratory desorption experiment on filter-collected atmospheric particles. They found that 6 of the 9 PAH's measured (acenaphthene, acenaphthylene,

benz(a)anthracene, chrysene, fluoranthene, 2-methyl phenanthrene, and pyrene) were more or less fully exchangeable, but, the time scales for vapor/particle exchange (including intraparticle diffusion) in their experiments were much longer than those predicted by Rounds and Pankow (1990). Based on these results, they concluded that for the PAH's considered, vapor/particle equilibrium may not be achieved in the atmosphere, even for PAH's that are fully exchangeable. Three of the PAH's measured had apparently non-exchangeable particle-associated fractions: phenanthrene, fluorene, and 9-fluorenone.

One interesting question that has been raised by this analysis concerns the phase distribution of cadmium in the atmosphere. Cadmium is generally assumed to be associated with particles in the atmosphere, although it can be in the vapor phase in combustion and incineration processes. The simplified vapor/particle partitioning analysis conducted in this study *suggests* that there may be some cadmium in the vapor phase in the atmosphere under certain conditions, but, this is very uncertain. Cadmium melts at about 321 °C and is a relatively volatile metal. While it is more volatile than many metals, it is not nearly as volatile as mercury. Cadmium has a vapor pressure on the order of 10,000 - 100,000 times lower than mercury at the same temperature; a crude estimate of the saturation vapor pressure of pure cadmium metal at 25 °C is of the order of 1e-12 atm ( $1 \times 10^{-12}$  atm). (Vapor pressure data and estimates are shown in the figure below.) If this is "correct", its vapor pressure at 25 °C is similar to that of 2,3,7,8-TCDD, a compound that is predicted to exist in both the vapor and particle phases in the atmosphere, depending intimately on the micro-meteorological conditions. Of course, different cadmium compounds have different vapor pressures, and, the form of cadmium in the atmosphere may play an important role. Cadmium oxide and cadmium chloride, for example, have much lower vapor pressures than pure cadmium metal.

## Vapor Pressure Data for Some Metals and Metallic Compounds



Data from CRC Handbook of Chemistry and Physics, 56th Edition, 1975-6

## **Appendix C.2.**

### **Results of Vapor/Particle Partitioning Estimates**

In the table below, results are given for vapor/particle partitioning calculations -- using the theory described in Appendix C.1. above -- for the compounds considered in this analysis.

## Vapor/Particle Partitioning Estimates

NAME	Vapor/Particle Partitioning Estimates				
		low end of fraction adsorbed range T = 310K sa=4.2e-7 cm <sup>2</sup> /cm <sup>3</sup>	middle of fraction adsorbed range T = 290K sa=3.5e-6 cm <sup>2</sup> /cm <sup>3</sup>	high end of fraction adsorbed range T = 260K sa=1.1e-5 cm <sup>2</sup> /cm <sup>3</sup>	
	IUPAC #	values from calc	values from calc	values from calc	
	CAS # (1)				
common chemical name					
octachlorostyrene	029082-74-4	1.5E-004	2.8E-003	3.8E-002	
4-bromophenyl phenyl ether	000101-55-3	1.7E-005	5.2E-004	1.7E-002	
3,3'-dichlorobenzidine	000091-94-1	2.9E-001	9.0E-001	9.9E-001	
1,3-dinitropyrene	075321-20-9	2.8E-002	3.5E-001	8.8E-001	
1,6-dinitropyrene	042397-64-8	2.8E-002	3.5E-001	8.8E-001	
1,8-dinitropyrene	042397-65-9	2.8E-002	3.5E-001	8.8E-001	
2,7-dinitropyrene	117929-15-4	2.8E-002	3.5E-001	8.8E-001	
dinitropyrenes (mixed)	078432-19-6	2.8E-002	3.5E-001	8.8E-001	
hexachloro-1,3-butadiene	000087-68-3	1.9E-007	4.8E-006	1.1E-004	
4,4'-methylene bis(2-chloroaniline)	000101-14-4	4.7E-004	9.4E-003	1.3E-001	
pentachlorophenol	000087-86-5	4.1E-005	6.4E-004	6.2E-003	
aldrin	000309-00-2	4.4E-005	9.2E-004	1.5E-002	
ieldrin	000060-57-1	2.0E-004	3.3E-003	3.4E-002	
p,p'-DDT	000050-29-3	2.5E-002	2.9E-001	7.9E-001	
p,p'-DDD	000072-54-8	5.1E-003	8.8E-002	5.7E-001	
p,p'-DDE	000072-55-9	1.3E-003	2.4E-002	2.5E-001	
heptachlor	000076-44-8	1.8E-005	3.1E-004	3.8E-003	
heptachlor epoxide	001024-57-3	1.2E-004	1.9E-003	1.9E-002	
methoxychlor	000072-43-5	5.4E-003	9.5E-002	6.0E-001	
mirex	002385-85-5	1.1E-006	2.4E-005	4.7E-004	
toxaphene	008001-35-2	3.8E-003	1.1E-001	7.9E-001	
endrin	000072-20-8	7.1E-005	1.4E-003	2.0E-002	
alpha-hexachlorocyclohexane	000319-84-6	4.0E-005	6.1E-004	5.6E-003	
beta-hexachlorocyclohexane	000319-85-7	1.3E-004	1.6E-003	1.0E-002	
delta-hexachlorocyclohexane	000319-86-8	7.3E-005	1.2E-003	1.3E-002	
gamma-hexachlorocyclohexane	000058-89-9	1.6E-004	2.8E-003	3.3E-002	
mixed hexachlorocyclohexanes	000319-84-6				

## Vapor/Particle Partitioning Estimates

<b>Vapor/Particle Partitioning Estimates</b>					
<b>NAME</b>	IUPAC #	cas # (1)	low end	middle	high end
			of fraction	of fraction	of fraction
			adsorbed	adsorbed	adsorbed
			range	range	range
			T = 310K	T = 290K	T = 260K
			sa=4.2e-7 cm <sup>2</sup> /cm <sup>3</sup>	sa=3.5e-6 cm <sup>2</sup> /cm <sup>3</sup>	sa=1.1e-5 cm <sup>2</sup> /cm <sup>3</sup>
			values from calc	values from calc	values from calc
cadmium	007440-43-9		8.0E-001	1.0E+000	1.0E+000
cadmium carbonate	000513-78-0				
cadmium chloride	010108-64-2		1.0E+000	1.0E+000	1.0E+000
cadmium oxide	001306-19-0				
cadmium sulfate	010124-36-4				
cadmium sulfide	001306-23-6				
elemental mercury	007439-97-6		1.4E-005	4.8E-004	1.8E-002
mercury oxide	021908-53-2				
mercuric chloride	007487-94-7		2.7E-008	3.6E-007	2.6E-006
monomethyl mercury chloride	000115-09-3		1.5E-007	2.8E-006	3.8E-005
dimethyl mercury	000593-74-8				
tetraethyl lead	000078-00-2		7.4E-008	1.8E-006	4.1E-005
tetramethyl lead	000075-74-1		8.6E-010	2.5E-008	7.0E-007
triethyl lead radical (1+ cation)	014570-15-1				
triethyl lead hydride	005224-23-7				
triethyl lead chloride	001067-14-7				
diethyl lead radical (2+ cation)	024952-65-6				
diethyl lead dihydride	081494-11-3				
diethyl lead dichloride	013231-90-8				
trimethyl lead radical (1+ cation)	014570-16-2				
trimethyl lead hydride	007442-13-9				
trimethyl lead chloride	001520-78-1				
dimethyl lead radical (2+ cation)	021774-13-0				
dimethyl lead dihydride	030691-92-0				
dimethyl lead dichloride	001520-77-0				
bis (tributyltin) oxide	000056-35-9		2.4E-002	4.8E-001	9.8E-001
tributyl tin	000688-75-3				
tributyltin fluoride	001983-10-4				
tributyltin chloride	001461-22-9				
tributyltin hydroxide	001067-97-6				
tributyltin naphthenate					
tris(tributylstannyl) phosphate	013435-05-7				

## Vapor/Particle Partitioning Estimates

NAME	IUPAC #	cas # (1)	Vapor/Particle Partitioning Estimates		
			low end of fraction adsorbed range T = 310K sa=4.2e-7 cm2/cm3	middle of fraction adsorbed range T = 290K sa=3.5e-6 cm2/cm3	high end of fraction adsorbed range T = 260K sa=1.1e-5 cm2/cm3
			values from calc	values from calc	values from calc
1,4-dichlorobenzene	000106-46-7		3.1E-008	4.4E-007	3.4E-006
1,2,3,4-tetrachlorobenzene	000634-66-2		5.6E-007	9.3E-006	1.0E-004
1,2,4,5-tetrachlorobenzene	000095-94-3		5.4E-007	7.7E-006	6.3E-005
1,2,3,5-tetrachlorobenzene	000634-90-2		2.6E-007	4.2E-006	4.4E-005
pentachlorobenzene	000608-93-5		5.5E-006	9.2E-005	1.0E-003
hexachlorobenzene	000118-74-1		2.1E-005	3.1E-004	2.8E-003
naphthalene	000091-20-3		1.4E-007	2.1E-006	1.8E-005
acenaphthene	000083-32-9		3.2E-006	5.3E-005	5.6E-004
acenaphthylene	000208-96-8		1.2E-006	1.9E-005	2.0E-004
fluorene	000086-73-7		6.8E-006	1.1E-004	1.2E-003
phenanthrene	000085-01-8		4.0E-005	7.5E-004	1.0E-002
anthracene	000120-12-7		6.4E-005	1.0E-003	9.9E-003
pyrene	000129-00-0		3.9E-004	7.0E-003	8.2E-002
fluoranthene	000206-44-0		5.0E-004	9.9E-003	1.3E-001
chrysene	000218-01-9		4.0E-002	4.4E-001	9.2E-001
benz [ a ] anthracene	000056-55-3		4.6E-002	5.0E-001	9.4E-001
benzo [ b ] fluoranthene	000205-99-2		2.3E-003	5.1E-002	5.2E-001
benzo [ j ] fluoranthene	000205-82-3		7.5E-002	6.5E-001	9.7E-001
benzo [ k ] fluoranthene	000207-08-9		5.0E-001	9.6E-001	1.0E+000
benzo [ a ] pyrene	000050-32-8		1.6E-001	8.2E-001	9.9E-001
benzo [ e ] pyrene	000192-97-2		1.3E-001	8.1E-001	9.9E-001
perylene	000198-55-0		5.0E-001	9.5E-001	1.0E+000
benzo [ g,h,i ] perylene	000191-24-2		4.9E-001	9.6E-001	1.0E+000
dibenz [a,h] anthracene	000053-70-3		9.8E-001	1.0E+000	1.0E+000
indeno [ 1,2,3-c,d ] pyrene	000193-39-5		8.8E-001	9.9E-001	1.0E+000

## Vapor/Particle Partitioning Estimates

<b>Vapor/Particle Partitioning Estimates</b>					
<b>NAME</b>	IUPAC #	cas # (1)	low end	middle	high end
			of fraction	of fraction	of fraction
			adsorbed	adsorbed	adsorbed
			range	range	range
			T = 310K	T = 290K	T = 260K
			sa=4.2e-7 cm <sup>2</sup> /cm <sup>3</sup>	sa=3.5e-6 cm <sup>2</sup> /cm <sup>3</sup>	sa=1.1e-5 cm <sup>2</sup> /cm <sup>3</sup>
common chemical name	IUPAC #	cas # (1)	values from calc	values from calc	values from calc
2,3,7,8-TCDD	001746-01-6		7.5E-002	5.9E-001	9.4E-001
1,2,3,7,8-PeCDD	040321-76-4		5.0E-001	9.6E-001	1.0E+000
1,2,3,4,7,8-HxCDD	039227-28-6		7.5E-001	9.8E-001	1.0E+000
1,2,3,6,7,8-HxCDD	057653-85-7		7.5E-001	9.8E-001	1.0E+000
1,2,3,7,8,9-HxCDD	019408-74-3		7.5E-001	9.8E-001	1.0E+000
1,2,3,4,6,7,8-HpCDD	035822-46-9		9.6E-001	1.0E+000	1.0E+000
OCDD	003268-87-9		9.8E-001	1.0E+000	1.0E+000
2,3,7,8-TCDF	051207-31-9		2.2E-002	3.0E-001	8.6E-001
2,3,4,7,8-PeCDF	057117-31-4		2.0E-001	8.4E-001	9.9E-001
1,2,3,7,8-PeCDF	057117-41-6		2.0E-001	8.4E-001	9.9E-001
1,2,3,4,7,8-HxCDF	070648-26-9		5.8E-001	9.7E-001	1.0E+000
1,2,3,6,7,8-HxCDF	057117-44-9		5.2E-001	9.6E-001	1.0E+000
1,2,3,7,8,9-HxCDF	072918-21-9		5.5E-001	9.6E-001	1.0E+000
2,3,4,6,7,8-HxCDF	060851-34-5		5.5E-001	9.6E-001	1.0E+000
1,2,3,4,6,7,8-HpCDF	067562-39-4		8.8E-001	9.9E-001	1.0E+000
1,2,3,4,7,8,9-HpCDF	055673-89-7		8.8E-001	9.9E-001	1.0E+000
OCDF	039001-02-0		9.8E-001	1.0E+000	1.0E+000

## Vapor/Particle Partitioning Estimates

		Vapor/Particle Partitioning Estimates				
NAME			low end of fraction adsorbed range T = 310K sa=4.2e-7 cm <sup>2</sup> /cm <sup>3</sup>	middle of fraction adsorbed range T = 290K sa=3.5e-6 cm <sup>2</sup> /cm <sup>3</sup>	high end of fraction adsorbed range T = 260K sa=1.1e-5 cm <sup>2</sup> /cm <sup>3</sup>	
common chemical name	IUPAC #	cas # (1)	values from calc	values from calc	values from calc	
biphenyl	0	000092-52-4	1.33E-006	2.16E-005	2.24E-004	
2-PCB	1	002051-60-7	1.4E-006	6.6E-005	4.5E-003	
3-PCB	2	002051-61-8	2.6E-006	1.3E-004	9.8E-003	
4-PCB	3	002051-62-9	2.8E-006	1.4E-004	1.0E-002	
count			3	3	3	
average			<b>2.27E-006</b>	<b>1.11E-004</b>	<b>8.25E-003</b>	
standard deviation			6.14E-007	3.24E-005	2.67E-003	
minimum			<b>1.40E-006</b>	6.56E-005	4.48E-003	
maximum			2.76E-006	1.37E-004	<b>1.04E-002</b>	
2,2'-PCB	4	013029-08-8	7.5E-006	4.1E-004	3.5E-002	
2,3-PCB	5	016605-91-7	1.6E-005	9.3E-004	8.4E-002	
2,4-PCB	7	033284-50-3	1.3E-005	7.5E-004	7.4E-002	
2,4'-PCB	8	034883-43-7	1.5E-005	8.6E-004	7.9E-002	
2,5-PCB	9	034883-39-1	1.3E-005	7.5E-004	7.5E-002	
2,6-PCB	10	033146-45-1	7.4E-006	4.0E-004	3.4E-002	
3,3'-PCB	11	002050-67-1	2.6E-005	1.6E-003	1.6E-001	
3,4-PCB	12	002974-92-7	3.0E-005	1.8E-003	1.7E-001	
3,5-PCB	14	034883-41-5	1.8E-005	1.1E-003	1.1E-001	
4,4'-PCB	15	002050-68-2	3.1E-005	2.0E-003	1.9E-001	
count			10	10	10	
average			<b>1.76E-005</b>	<b>1.06E-003</b>	<b>1.01E-001</b>	
standard deviation			8.11E-006	5.30E-004	5.17E-002	
minimum			<b>7.38E-006</b>	3.97E-004	3.39E-002	
maximum			3.08E-005	1.96E-003	<b>1.90E-001</b>	

## Vapor/Particle Partitioning Estimates

<b>Vapor/Particle Partitioning Estimates</b>					
<b>NAME</b>			low end	middle	high end
			of fraction	of fraction	of fraction
			adsorbed	adsorbed	adsorbed
			range	range	range
			T = 310K	T = 290K	T = 260K
			sa=4.2e-7 cm <sup>2</sup> /cm <sup>3</sup>	sa=3.5e-6 cm <sup>2</sup> /cm <sup>3</sup>	sa=1.1e-5 cm <sup>2</sup> /cm <sup>3</sup>
common chemical name	IUPAC #	cas # (1)	values from calc	values from calc	values from calc
2,2',3-PCB	16	038444-78-9	4.2E-005	2.6E-003	2.3E-001
2,2',5-PCB	18	037680-65-2	2.9E-005	1.8E-003	1.7E-001
2,3,3'-PCB	20	038444-84-7	7.7E-005	5.1E-003	4.0E-001
2,3,4-PCB	21	055702-46-0	7.8E-005	5.2E-003	4.1E-001
2,3',5-PCB	26	038444-85-8	5.3E-005	3.6E-003	3.2E-001
2,4,4'-PCB	28	007012-37-5	6.4E-005	4.3E-003	3.6E-001
2,4,5-PCB	29	015862-07-4	5.0E-005	3.2E-003	2.8E-001
2,4,6-PCB	30	035693-92-6	2.4E-005	1.4E-003	1.4E-001
2,4',5,-PCB	31	016606-02-3	7.9E-005	5.3E-003	4.1E-001
2',3,4-PCB	33	038444-86-9	8.2E-005	5.5E-003	4.2E-001
3,3',4-PCB	35	037680-69-6	1.5E-004	1.1E-002	6.3E-001
3,4,4'-PCB	37	038444-90-5	1.6E-004	1.2E-002	6.5E-001
<hr/>					
count			12	12	12
average			<b>7.42E-005</b>	<b>5.05E-003</b>	<b>3.68E-001</b>
standard deviation			4.13E-005	3.09E-003	1.50E-001
minimum			<b>2.37E-005</b>	1.44E-003	1.38E-001
maximum			1.63E-004	1.18E-002	<b>6.47E-001</b>
<hr/>					
2,2',3,3'-PCB	40	038444-93-8	2.1E-004	1.5E-002	7.1E-001
2,2',3,5'-PCB	44	041464-39-5	1.6E-004	1.2E-002	6.4E-001
2,2',4,4'-PCB	47	002437-79-8	1.4E-004	9.7E-003	6.0E-001
2,2',4,5'-PCB	49	041464-40-8	1.2E-004	8.9E-003	5.8E-001
2,2',4,6-PCB	50	062796-65-0	2.5E-003	4.2E-002	3.5E-001
2,2',4,6'-PCB	51	068194-04-7	8.7E-005	5.9E-003	4.5E-001
2,2,5,5'-PCB	52	035693-99-3	1.3E-004	9.3E-003	5.8E-001
2,2,5,6'-PCB	53	041464-41-9	7.8E-005	5.3E-003	4.2E-001
2,2,6,6'-PCB	54	015968-05-5	6.2E-005	3.5E-003	2.6E-001
2,3,4,4'-PCB	60	033025-41-1	3.8E-004	2.9E-002	8.4E-001
2,3,4,5-PCB	61	033284-53-6	1.6E-004	1.3E-002	6.9E-001
2,3,5,6-PCB	65	033284-54-7	1.5E-004	1.1E-002	6.2E-001
2,3,4,4'-PCB	66	032598-10-0	3.2E-004	2.4E-002	8.1E-001
2,3',4,5-PCB	70	032598-11-1	3.6E-004	2.8E-002	8.4E-001
2,4,4',6-PCB	75	032598-12-2	1.2E-004	8.3E-003	5.6E-001
3,3',4,4'-PCB	77	032598-13-3	8.6E-004	6.9E-002	9.4E-001
3,3',5,5'-PCB	80	033284-52-5	3.4E-004	2.9E-002	8.6E-001
3,4,4',5-PCB	81	070362-50-4	6.5E-004	5.4E-002	9.2E-001
<hr/>					
count			18	18	18
average			<b>3.77E-004</b>	<b>2.09E-002</b>	<b>6.48E-001</b>
standard deviation			5.49E-004	1.77E-002	1.92E-001
minimum			<b>6.16E-005</b>	3.49E-003	2.55E-001
maximum			2.48E-003	6.85E-002	<b>9.37E-001</b>

## Vapor/Particle Partitioning Estimates

<b>Vapor/Particle Partitioning Estimates</b>					
<b>NAME</b>			low end	middle	high end
			of fraction	of fraction	of fraction
			adsorbed	adsorbed	adsorbed
			range	range	range
			T = 310K	T = 290K	T = 260K
			sa=4.2e-7 cm <sup>2</sup> /cm <sup>3</sup>	sa=3.5e-6 cm <sup>2</sup> /cm <sup>3</sup>	sa=1.1e-5 cm <sup>2</sup> /cm <sup>3</sup>
common chemical name	IUPAC #	cas # (1)	values from calc	values from calc	values from calc
2,2',3,3',5-PCB	83	060145-20-2	7.0E-004	5.6E-002	9.2E-001
2,2',3,4,5-PCB	86	065510-45-4	6.9E-004	5.5E-002	9.2E-001
2,2,3,4,5'-PCB	87	038380-02-8	8.2E-004	6.6E-002	9.4E-001
2,2',3,4,6-PCB	88	055215-17-3	3.3E-004	2.6E-002	8.2E-001
2,2',3,5,6-PCB	95	038379-99-6	3.7E-004	2.9E-002	8.4E-001
2,2',4,4',5-PCB	99	038380-01-7	6.3E-004	5.1E-002	9.2E-001
2,2,4,4',6-PCB	100	039485-83-1	1.2E-002	2.5E-001	8.9E-001
2,2,4,5,5'-PCB	101	037680-73-2	5.6E-004	4.5E-002	9.0E-001
2,2',4,6,6'-PCB	104	056558-16-8	7.0E-004	5.6E-002	9.2E-001
2,3,3',4,4'-PCB	105	032598-14-4	2.0E-003	1.6E-001	9.8E-001
2,3,3',4,6-PCB	110	038380-03-9	1.0E-003	8.1E-002	9.5E-001
2,3,4,4',5-PCB	114	074472-37-0	1.4E-003	1.2E-001	9.7E-001
2,3,4,5,6-PCB	116	018259-05-7	8.2E-004	6.5E-002	9.3E-001
2,3',4,4',5-PCB	118	031508-00-6	1.5E-003	1.2E-001	9.7E-001
2',3,4,5,5'-PCB	124	070424-70-3	2.3E-003	1.7E-001	9.8E-001
3,3',4,4',5-PCB	126	057465-28-8	3.4E-003	2.7E-001	9.9E-001
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count			16	16	16
average			<b>1.87E-003</b>	<b>1.01E-001</b>	<b>9.27E-001</b>
standard deviation			2.86E-003	7.27E-002	4.64E-002
minimum			<b>3.31E-004</b>	2.56E-002	8.23E-001
maximum			1.25E-002	2.66E-001	<b>9.91E-001</b>
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2,2',3,3',4,4'-PCB	128	038380-07-3	4.9E-003	3.3E-001	9.9E-001
2,2',3,3',4,5-PCB	129	055215-18-4	3.9E-003	2.8E-001	9.9E-001
2,2',3,3',5,6-PCB	134	052704-70-8	1.5E-003	1.2E-001	9.7E-001
2,2',3,3',6,6'-PCB	136	038411-22-2	1.3E-003	8.9E-002	9.4E-001
2,2',3,4,4',5-PCB	138	035065-28-2	3.4E-003	2.5E-001	9.9E-001
2,2',3,4',5,6-PCB	149	038380-04-0	1.6E-003	1.3E-001	9.7E-001
2,2',4,4',5,5'-PCB	153	035065-27-1	2.6E-003	2.0E-001	9.8E-001
2,2',4,4',6,6'-PCB	155	033979-03-2	5.2E-004	3.8E-002	8.7E-001
2,3,3',4,4',5-PCB	156	038380-08-4	7.6E-003	4.5E-001	1.0E+000
2,3,3',4,4',5'-PCB	157	069782-90-7	8.2E-003	4.7E-001	1.0E+000
2,3',4,4',5,5'-PCB	167	052663-72-6	5.8E-003	3.9E-001	9.9E-001
3,3',4,4',5,5'-PCB	169	032774-16-6	2.2E-002	7.4E-001	1.0E+000
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count			12	12	12
average			<b>5.31E-003</b>	<b>2.90E-001</b>	<b>9.74E-001</b>
standard deviation			5.65E-003	1.92E-001	3.65E-002
minimum			<b>5.25E-004</b>	3.81E-002	8.65E-001
maximum			2.23E-002	7.43E-001	<b>9.99E-001</b>

## Vapor/Particle Partitioning Estimates

<b>Vapor/Particle Partitioning Estimates</b>					
<b>NAME</b>			low end	middle	high end
			of fraction	of fraction	of fraction
			adsorbed	adsorbed	adsorbed
			range	range	range
			T = 310K	T = 290K	T = 260K
			sa=4.2e-7 cm <sup>2</sup> /cm <sup>3</sup>	sa=3.5e-6 cm <sup>2</sup> /cm <sup>3</sup>	sa=1.1e-5 cm <sup>2</sup> /cm <sup>3</sup>
common chemical name	IUPAC #	cas # (1)	values from calc	values from calc	values from calc
2,2',3,3',4,4',5-PCB	170	035065-30-6	1.8E-002	6.8E-001	1.0E+000
2,2',3,3',4,4',6-PCB	171	052663-71-5	8.7E-003	4.9E-001	1.0E+000
2,2',3,4,4',5,5'-PCB	180	035065-29-3	1.2E-002	5.8E-001	1.0E+000
2,2',3,4,5,5',6-PCB	185	052712-05-7	5.2E-003	3.5E-001	9.9E-001
2,2',3,4',5,5',6-PCB	187	052663-68-0	5.5E-003	3.6E-001	9.9E-001
2,3,3',4,4',5,5'-PCB	189	039635-31-9	3.0E-002	8.0E-001	1.0E+000
count			6	6	6
average			<b>1.34E-002</b>	<b>5.44E-001</b>	<b>9.97E-001</b>
standard deviation			8.80E-003	1.61E-001	2.17E-003
minimum			<b>5.17E-003</b>	3.55E-001	9.94E-001
maximum			3.04E-002	7.98E-001	<b>9.99E-001</b>
2,2',3,3',4,4',5,5'-PCB	194	035694-08-7	6.7E-002	9.0E-001	1.0E+000
2,2',3,3',5,5',6,6'-PCB	202	002136-99-4	3.3E-003	2.5E-001	9.9E-001
count			2	2	2
average			<b>3.51E-002</b>	<b>5.76E-001</b>	<b>9.94E-001</b>
standard deviation			3.18E-002	3.28E-001	5.49E-003
minimum			<b>3.28E-003</b>	2.48E-001	9.89E-001
maximum			6.69E-002	9.05E-001	<b>1.00E+000</b>
2,2',3,3',4,4',5,5',6-PCB	206	040186-72-9	1.2E-001	9.5E-001	1.0E+000
2,2',3,3',4,4',5,6,6'-PCB	207	052663-79-3	4.8E-002	8.5E-001	1.0E+000
2,2',3,3',4,5,5',6,6'-PCB	208	052663-77-1	5.0E-002	8.6E-001	1.0E+000
count			3	3	3
average			<b>7.08E-002</b>	<b>8.86E-001</b>	<b>1.00E+000</b>
standard deviation			3.15E-002	4.43E-002	1.81E-004
minimum			<b>4.75E-002</b>	8.52E-001	9.99E-001
maximum			1.15E-001	9.49E-001	<b>1.00E+000</b>
2,2',3,3',4,4',5,5',6,6'-PCB	209	002051-24-3	9.38E-002	9.32E-001	1.00E+000

### **Appendix C.3.**

#### **Comparison of Vapor/Particle Partitioning Estimates with Examples of Vapor/Particle Partitioning Measurements from the Literature**

As described in Appendix C.1. and presented in Appendix C.2., above, estimates were made using the adsorption-based theory of Junge (1977), with the subcooled liquid-phase vapor pressure substituted for the solid phase vapor pressure, as recommended by Bidleman (1988).

The central estimates of this analysis — shown in the table below in bold face — were carried out using a temperature of 290 °K (~17 °C; ~62 °F). An aerosol surface area of  $3.5 \times 10^{-6} \text{ cm}^2$  aerosol surface area per  $\text{cm}^3$  of air ( $\text{cm}^2/\text{cm}^3$ ) was selected, corresponding to the “background + local sources” aerosol surface area category (Whitby, 1978; Bidleman, 1988). In addition to the physical-chemical properties of the pollutant in question, vapor/particle partitioning depends intimately on local meteorological conditions and on the local nature of the atmospheric aerosol.

In order to gain some perspective on the range of vapor/particle partitioning that might be encountered, estimates were also made for a scenarios in which adsorption to particles was at the low and high ends of the expected environmental range.

For the estimated low end of the expected particle-adsorbed range, a relatively high temperature was selected, and a relatively low aerosol surface area was assumed. The conditions chosen were a temperature of 310 °K (~37 °C; ~98 °F) and an aerosol surface area of  $4.2 \times 10^{-7} \text{ cm}^2/\text{cm}^3$ . This surface area corresponds to the “clean continental background” aerosol surface area category (Whitby, 1978; Bidleman, 1988).

For the estimated high end of the expected particle-adsorbed range, a relatively low temperature was selected, and a relatively high aerosol surface area was assumed. The conditions chosen were a temperature of 260 °K (~ -13 °C; ~8 °F) and an aerosol surface area of  $1.1 \times 10^{-5} \text{ cm}^2/\text{cm}^3$ . This surface area corresponds to the “urban” aerosol surface area category (Whitby, 1978; Bidleman, 1988). [Note: the global mean temperature at a height of 4000 meters is estimated to be on the order of 262 °K (Ballschmiter and Wittlinger, 1991)].

In Table C.3.-(1) below, the results of these estimates are presented, along with examples of information from the literature regarding vapor/particle partitioning of the selected compounds in the atmosphere.

The range of the above conditions is rather large, but, for many of the compounds considered in this analysis, their physical chemical properties suggest that they will reside predominantly in the vapor phase (e.g., hexachlorobenzene) or the particle phase (e.g., OCDD) under most ambient conditions. Some of the compounds, however, are predicted to vary quite significantly over the above range of conditions. For example, in the “central” partitioning scenario, approximately 60% of atmospheric 2,3,7,8-TCDD is estimated to associated with the particle phase; for the high and low scenarios considered, the estimated fraction-adsorbed ranges from 8% to 90%.

**Table C.3.-(1). Vapor Particle Partitioning Summary  
for Compounds Considered in this Study**

Chemical or Group	Level	Estimated Fraction Adsorbed to Particle Phase in Atmosphere Based on Calculations in Appendix C [Central Estimate ( <b>bold</b> ) T = 290 °K; Aerosol surface area = 3.5e-6 cm <sup>2</sup> /cm <sup>3</sup> ] [RANGE (in parentheses): 310 to 260 °K; 4.2e-7 to 1.1e-5 cm <sup>2</sup> /cm <sup>3</sup> ]	Examples from the Literature of Information Regarding Vapor/Particle Partitioning		
			fraction adsorbed to atmospheric particles	Temperature (°C)	Reference (see end of Table)
<b>METALS / ORGANOMETALLICS</b>					
<b>Alkylated Lead</b> TEL = Tetraethyl Lead TML = Tetramethyl Lead	I	<b>0.000002</b> (TEL) (0.0000007 - 0.00004)	< 0.00003		13
		<b>0.00000003</b> (TML) (1e-9 - 0.00004)	< 0.00001		13
<b>Mercury</b>	I	<b>0.0005</b> (Hg) (0.00001 - 0.02)	... it is now known that only a few percent of the total airborne Hg is in the particulate phase. The major chemical form(s) of Hg associated with atmospheric aerosols have so far not been identified .” (11)		
		<b>0.0000004</b> (HgCl <sub>2</sub> ) (0.0000003 - 0.00003)	“Currently it is felt that Hg(p) contributes a small (<5%) fraction of the total amount of Hg found in the ambient air.” Several studies at sites in the Great Lakes region are cited showing a range of particulate fraction of total Hg to be (12): 0.006 - 0.023 (over Lake Michigan); 0.001 - 0.073 (Chicago, IL); 0.007 - 0.117 (South Haven, MI); 0.003 - 0.126 (Chicago, IL); 0.020 - 0.162 (South Haven, MI); 0.003 - 0.200 (Ann Arbor, MI); 0.001 - 0.410 (Detroit, MI)		
		<b>0.000003</b> (HgCH <sub>3</sub> Cl) (0.0000002 - 0.00004)			
<b>Cadmium</b>	II	<b>1</b> (Cd) (0.8 - 1)	Cadmium is generally assumed to be associated with particles in the atmosphere, although it can be in the vapor phase in combustion and incineration processes. The simplified vapor/particle partitioning analysis conducted in this study suggests that there may be a small amount of cadmium in the vapor phase in the atmosphere under certain conditions, but, this is very uncertain. Additional details are given in Appendix C, in the discussion of vapor/particle partitioning.		
		<b>1</b> (CdCl <sub>2</sub> )			
<b>Tributyltin</b> TBTO = Tributyltin Oxide	II	<b>0.5</b> (TBTO) (0.02 - 0.98)	If released to the atmosphere, TBTO can be expected to exist in both the particle phase and the vapor phase in the ambient atmosphere (14)  The ATSDR Toxicological Profile for Tin (1992) reports that no information on tributyltin compounds in the ambient atmosphere is available.  In general, no information on tributyltin compounds in the atmosphere could be found. Measurements of tin in the atmosphere generally measure only the total tin content, and do not attempt to speciate the tin compounds.		

**Table C.3.-(1). Vapor Particle Partitioning Summary  
for Compounds Considered in this Study**

Chemical or Group	Level	Estimated Fraction Adsorbed to Particle Phase in Atmosphere Based on Calculations in Appendix C [Central Estimate ( <b>bold</b> ) T = 290°K; Aerosol surface area = 3.5e-6 cm <sup>2</sup> /cm <sup>3</sup> ] [RANGE (in parentheses): 310 to 260 °K; 4.2e-7 to 1.1e-5 cm <sup>2</sup> /cm <sup>3</sup> ]	Examples from the Literature of Information Regarding Vapor/Particle Partitioning		
			fraction adsorbed to atmospheric particles	Temperature (°C)	Reference (see end of Table)
<b>ORGANOCHLORINE BIOCIDES</b>					
Aldrin / Dieldrin	I	<b>0.0009</b> (Aldrin) (0.00004 - 0.02)			
		<b>0.003</b> (Dieldrin) (0.0002 - 0.03)			
DDT / DDD / DDE	I	<b>0.3</b> (DDT) (0.03 - 0.8)	<b>0.73 - 0.88</b> <b>0.089 - 0.74</b>	-5.9 to 1.8 0 - 20	1 4
		<b>0.09</b> (DDD) (0.005 - 0.6)			
		<b>0.02</b> (DDE) (0.001 - 0.3)	<b>0.18 - 0.41</b> ≤ <b>0.03</b> <b>0.05</b> (avg) <b>0.02 - 0.24</b>	-5.9 to 1.8 8 - 26 20 - 28 0 - 20	1 2 3 4
Mirex	I	<b>0.00002</b> (0.000001 - 0.0005)			
Toxaphene	I	<b>0.1</b> (0.004 - 0.8)			
Endrin	II	<b>0.001</b> (0.00007 - 0.02)			
Heptachlor / Heptachlor Epoxide	II	<b>0.0003</b> Hept. (0.00002 - 0.004)			
		<b>0.002</b> Hept. Epox. (0.0001 - 0.02)			
Hexachloro-cyclohexane	II	<b>0.0006</b> (α) (0.00004 - 0.006)	<b>0.0008 - 0.004</b>	0 - 20	4
		<b>0.002</b> (β) (0.0001 - 0.01)			
		<b>0.001</b> (δ) (0.00007 - 0.01)			
		<b>0.003</b> (γ) (0.0002 - 0.03)			
Methoxychlor	II	<b>0.1</b> (0.005 - 0.6)			

**Table C.3.-(1). Vapor Particle Partitioning Summary  
for Compounds Considered in this Study**

Chemical or Group	Level	Estimated Fraction Adsorbed to Particle Phase in Atmosphere Based on Calculations in Appendix C [Central Estimate ( <b>bold</b> ) T = 290 °K; Aerosol surface area = 3.5e-6 cm <sup>2</sup> /cm <sup>3</sup> ] [RANGE (in parentheses): 310 to 260 °K; 4.2e-7 to 1.1e-5 cm <sup>2</sup> /cm <sup>3</sup> ]	Examples from the Literature of Information Regarding Vapor/Particle Partitioning		
			fraction adsorbed to atmospheric particles	Temperature (°C)	Reference (see end of Table)
Pentachlorophenol	II	<b>0.0006</b> (0.00004 - 0.006)			
<b>INDUSTRIAL / MISCELLANEOUS</b>					
Octachlorostyrene	I	<b>0.003</b> (0.0001 - 0.04)			
3,3'-Dichloro-benzidene	II	<b>0.9</b> (0.3 - 0.99)			
4,4'-Methylene bis (2-Chloroaniline) “MBOCA”	II	<b>0.009</b> (0.0005 - 0.1)			
4-Bromophenyl Phenyl Ether “4BPE”	II	<b>0.0005</b> (0.00002 - 0.02)			
Hexachloro-1,3-Butadiene “HCBD”	II	<b>0.000005</b> (0.0000002 - 0.0001)	“Hexachlorobutadiene can exist in the atmosphere as a vapor or adsorbed to airborne particulate matter... A high partition coefficient (Log Koc) value of 3.67 ... indicates that adsorption to soils with high organic content can occur. Wind erosion of contaminated surface soils can then lead to airborne hexachlorobutadiene-containing particulate matter. Levels of hexachlorobutadiene have been detected in flyash from the incineration of hexachlorobutadiene-containing hazardous waste (Junk and Ford 1980). The transport of particulate matter is a function of particle size and wind speed, however no data were located regarding the transport of hexachlorobutadiene particles in air.” (ATSDR-Hexachlorobutadiene, 1994)		

**Table C.3.-(1). Vapor Particle Partitioning Summary  
for Compounds Considered in this Study**

Chemical or Group	Level	Estimated Fraction Adsorbed to Particle Phase in Atmosphere Based on Calculations in Appendix C <small>[Central Estimate (<b>bold</b>) T = 290°K;            Aerosol surface area = 3.5e-6 cm<sup>2</sup>/cm<sup>3</sup>            [RANGE (in parentheses): 310 to 260 °K;            4.2e-7 to 1.1e-5 cm<sup>2</sup>/cm<sup>3</sup>]</small>	Examples from the Literature of Information Regarding Vapor/Particle Partitioning		
			fraction adsorbed to atmospheric particles	Temperature (°C)	Reference (see end of Table)
<b>CHLOROBENZENES</b>					
<b>1,4-dichlorobenzene</b> “pDCB”	II	<b>0.000004</b> (0.0000003 - 0.00003)			
<b>Tetrachlorobzenes</b> 1234 Tetrachlorobenzene 1245 Tetrachlorobenzene 1235 Tetrachlorobenzene  “1234TCB” “1245TCB” “1235TCB”	II	<b>0.000009</b> (1234TCB) (0.0000006 - 0.0001)			
		<b>0.000008</b> (1245TCB) (0.0000005 - 0.00006)			
		<b>0.000004</b> (1235TCB) (0.0000003 - 0.00004)			
<b>Pentachlorobenzene</b> “PeCB”	II	<b>0.00009</b> (0.000006 - 0.001)			
<b>Hexachlorobenzene</b> “HCB”	I	<b>0.0003</b> (0.00002 - 0.003)	<b>0.001 - 0.007</b>	0 - 20	4

**Table C.3.-(1). Vapor Particle Partitioning Summary  
for Compounds Considered in this Study**

Chemical or Group	Level	Estimated Fraction Adsorbed to Particle Phase in Atmosphere Based on Calculations in Appendix C [Central Estimate ( <b>bold</b> ) T = 290 °K; Aerosol surface area = 3.5e-6 cm <sup>2</sup> /cm <sup>3</sup> ] [RANGE (in parentheses): 310 to 260 °K; 4.2e-7 to 1.1e-5 cm <sup>2</sup> /cm <sup>3</sup> ]	Examples from the Literature of Information Regarding Vapor/Particle Partitioning		
			fraction adsorbed to atmospheric particles	Temperature (°C)	Reference (see end of Table)
<b>POLYCHLORINATED DIBENZO-P-DIOXINS AND DIBENZOFURANS (PCDD/F'S)</b>					
2,3,7,8-TCDD	I	<b>0.6</b> (0.08 - 0.9)	<b>0.13</b> avg for all samples: total TCDD	38 samples over 3 yrs; <3 °C: 11 samples 16-20 °C: 15 samples >28 °C: 12 samples	15
2,3,7,8-TCDF	I	<b>0.3</b> (0.02 - 0.9)	<b>0.09</b> avg for all samples: total TCDF	38 samples over 3 yrs; <3 °C: 11 samples 16-20 °C: 15 samples >28 °C: 12 samples	15
PeCDD/F's (pentachloro-)	I	<b>0.9</b> (0.2 - 0.99)	<b>0.36</b> avg for all samples: PeCDD/F's	38 samples over 3 yrs; <3 °C: 11 samples 16-20 °C: 15 samples >28 °C: 12 samples	15
HxCDD/F's (hexachloro-)	I	<b>0.97</b> (0.6 - 1)	<b>0.76</b> avg for all samples: total HxCDD/F's	38 samples over 3 yrs; <3 °C: 11 samples 16-20 °C: 15 samples >28 °C: 12 samples	15
HxCDD/F's (heptachloro-)	I	<b>0.99</b> (0.9 - 1)	<b>0.97</b> avg for all samples: total HpCDD/F's	38 samples over 3 yrs; <3 °C: 11 samples 16-20 °C: 15 samples >28 °C: 12 samples	15
OCDD/F's (octachloro-)	I	<b>1</b> (0.98 - 1)	<b>0.99</b> avg for all samples: total OCDD/F	38 samples over 3 yrs; <3 °C: 11 samples 16-20 °C: 15 samples >28 °C: 12 samples	15
PCDD/F's (as a group)	I		<b>~ 0.87</b> (avg) <b>0.54 - 0.74</b> <b>0.91 - 0.94</b> <b>0.31 - 0.56</b> <b>0.87 - 0.96</b> <b>0.74</b> (avg)	20 - 28  25 - 28 8 - 12  25 - 28 8 - 12  38 samples over 3 yrs; <3 °C: 11 samples 16-20 °C: 15 samples >28 °C: 12 samples	3  5 5  5 (TEQ) 5 (TEQ)  15

**Table C.3.-(1). Vapor Particle Partitioning Summary  
for Compounds Considered in this Study**

Chemical or Group	Level	Estimated Fraction Adsorbed to Particle Phase in Atmosphere Based on Calculations in Appendix C [Central Estimate ( <b>bold</b> ) T = 290°K; Aerosol surface area = 3.5e-6 cm <sup>2</sup> /cm <sup>3</sup> ] [RANGE (in parentheses): 310 to 260 °K; 4.2e-7 to 1.1e-5 cm <sup>2</sup> /cm <sup>3</sup> ]	Examples from the Literature of Information Regarding Vapor/Particle Partitioning		
			fraction adsorbed to atmospheric particles	Temperature (°C)	Reference (see end of Table)
<b>POLYCHLORINATED BIPHENYLS (PCB'S)</b>					
Cl <sub>1</sub> -PCB		<b>0.00007 - 0.00014</b> (0.000001 - 0.01)			
Cl <sub>2</sub> -PCB		<b>0.0004 - 0.0020</b> (0.000007 - 0.2)	< 0.01 (avg)	20 - 28	3
Cl <sub>3</sub> -PCB		<b>0.001 - 0.012</b> (0.00002 - 0.6)	< 0.001 (avg)	20 - 28	3
Cl <sub>4</sub> -PCB		<b>0.003 - 0.069</b> (0.00006 - 0.94)	<b>~ 0.024</b> (avg) <b>0.016 - 0.069</b> <b>0.11 - 0.22</b>	20 - 28 25 - 28 8 - 12	3 5 (coplanar) 5 (coplanar)
Cl <sub>5</sub> -PCB		<b>0.03 - 0.27</b> (0.0003 - 0.99)	n.d - 0.13 ~ 0.04 (avg) <b>0.03 - 0.04</b> <b>0.39 - 0.55</b>	-5.9 to 1.8 20 - 28 25 - 28 8 - 12	1 (PCB-101) 3 5 (coplanar) 5 (coplanar)
Cl <sub>6</sub> -PCB		<b>0.04 - 0.74</b> (0.0005 - 0.999)	n.d - 0.47 ~ 0.067 (avg) <b>0.02 - 0.41</b> <b>0.56 - 0.98</b>	-5.9 to 1.8 20 - 28 25 - 28 8 - 12	1 (PCB-153) 3 5 (coplanar) 5 (coplanar)
Cl <sub>7</sub> -PCB		<b>0.36 - 0.80</b> (0.005 - 0.999)	~ 0.2	20 - 28	3
Cl <sub>8</sub> -PCB		<b>0.25 - 0.91</b> (0.003 - 1.000)	~ 0.6	20 - 28	3
Cl <sub>9</sub> -PCB		<b>0.85 - 0.95</b> (0.05 - 1.000)			
Cl <sub>10</sub> -PCB		<b>0.93</b> (0.09 - 1.00)			
PCB's as a group	I		~ 0.04 <b>0.02 - 0.25</b>	20 - 28 0 - 20	3 4 (Arochlor 1254)

**Table C.3.-(1). Vapor Particle Partitioning Summary  
for Compounds Considered in this Study**

Chemical or Group	Level	Estimated Fraction Adsorbed to Particle Phase in Atmosphere Based on Calculations in Appendix C [Central Estimate ( <b>bold</b> ) T = 290°K; Aerosol surface area = 3.5e-6 cm <sup>2</sup> /cm <sup>3</sup> ] [RANGE (in parentheses): 310 to 260 °K; 4.2e-7 to 1.1e-5 cm <sup>2</sup> /cm <sup>3</sup> ]	Examples from the Literature of Information Regarding Vapor/Particle Partitioning		
			fraction adsorbed to atmospheric particles	Temperature (°C)	Reference (see end of Table)
<b>POLYCYCLIC AROMATIC HYDROCARBONS</b>					
Naphthalene “Naph”		<b>0.000002</b> (0.0000001 - 0.00002)	< 0.02	16	10-a
Acenaphthene “Acn”		<b>0.00005</b> (0.000003 - 0.0006)	< 0.02	16	10-a (Acn + Acl)
Acenaphthylene “Acl”		<b>0.00002</b> (0.000001 - 0.0002)	< 0.02	16	10-a (Acn + Acl)
Fluorene “Flr”		<b>0.0001</b> (0.000007 - 0.001)	~ 0 - 0.004 < 0.02 <b>0.0004 - 0.0166</b> <b>0.0039</b>	10 - 24 16 0 - 30 0 - 30	7 10-a 16(range) 16(median)
Phenanthrene “Phen”	II	<b>0.0008</b> (0.00004 - 0.01)	<b>0.003 - 0.007</b> <b>0.01</b> <b>&lt; 0.11</b> <b>0.08 +/- 0.02</b> <b>0.03 +/- 0.01</b> <b>0.0004 - 0.1025</b> <b>0.0103</b>	10 - 24 12 16 21 21 0 - 30 0 - 30	7 9 10-a 10-b 10-c 16(range) 16(median)
Anthracene “Anth”	II	<b>0.001</b> (0.00006 - 0.01)	< 0.03 <b>0.0006 - 0.97</b> <b>0.04</b>	16 0 - 30 0 - 30	10-a 16(range) 16(median)
Pyrene “Pyr”		<b>0.007</b> (0.0004 - 0.08)	<b>0.017 - 0.095</b> <b>0.01 - 0.29</b> <b>0.28</b> <b>0.15 +/- 0.07</b> <b>0.06 +/- 0.03</b> <b>0.005 - .520</b> <b>0.08</b>	10 - 24 5 - 29 12 21 21 0 - 30 0 - 30	7 8 9 10-b 10-c 16(range) 16(median)
Fluoranthene “Fln”		<b>0.01</b> (0.0005 - 0.1)	<b>0.012 - 0.082</b> <b>0.009 - 0.234</b> <b>0.28</b> <b>0.0014 - .4422</b> <b>0.064</b>	10 - 24 5 - 29 12 0 - 30 0 - 30	7 8 9 16(range) 16(median)
Chrysene “Chr”		<b>0.4</b> (0.04 - 0.9)	<b>0.97</b> <b>0.21 +/- 0.04</b> <b>0.15 +/- 0.03</b> <b>0.16 - 0.48</b>  <b>0.01 - ~ 1</b> <b>0.5</b>	12 21 21 10 - 24 0 - 30 0 - 30	9 10-b 10-c 7 (combined with triphenylene) 16(range) 16(median)

**Table C.3.-(1). Vapor Particle Partitioning Summary  
for Compounds Considered in this Study**

Chemical or Group	Level	Estimated Fraction Adsorbed to Particle Phase in Atmosphere Based on Calculations in Appendix C [Central Estimate ( <b>bold</b> ) T = 290°K; Aerosol surface area = 3.5e-6 cm <sup>2</sup> /cm <sup>3</sup> ] [RANGE (in parentheses): 310 to 260 °K; 4.2e-7 to 1.1e-5 cm <sup>2</sup> /cm <sup>3</sup> ]	Examples from the Literature of Information Regarding Vapor/Particle Partitioning		
			fraction adsorbed to atmospheric particles	Temperature (°C)	Reference (see end of Table)
Benz (a) Anthracene “BaA”	II	<b>0.5</b> (0.05 - 0.95)	~ 0.6 <b>0.023 - 0.67</b> 0.016 - ~1 0.87	4 - 13 10 - 24 0 - 30 0 - 30	6 7 16(range) 16(median)
Benzo (b) Fluoranthene “BbF”		<b>0.05</b> (0.002 - 0.5)	<b>0.35 - 0.57</b> 0.21 - ~1 0.93	10 - 24 0 - 20 0 - 30	7 16(range) 16(median)
Benzo (j) Fluoranthene “BjF”		<b>0.7</b> (0.08 - 0.97)			
Benzo (k) Fluoranthene “BkF”		<b>0.96</b> (0.5 - 1)	<b>0.34 - 0.52</b> .50 - ~1 ~ 1	10 - 24 0 - 30 0 - 30	7 16(range) 16(median)
Benzo (a) Pyrene “BaP”	I	<b>0.8</b> (0.2 - 0.99)	~1 <b>0.72 - 1.00</b> 0.8 - 1.0  <b>0.09 - ~1</b> ~1	-5.9 to 1.8 10 - 24 5 - 29  0 - 30 0 - 30	1 7 8 (BaP + BeP) 16(range) 16(median)
Benzo (e) Pyrene “BeP”		<b>0.8</b> (0.1 - 0.99)	0.8 - 1.0  <b>0.17 - ~1</b> 0.93	5 - 29  0 - 30 0 - 30	8 (BaP + BeP) 16(range) 16(median)
Perylene “Per”	II	<b>0.95</b> (0.5 - 1)			
Benzo (g,h,i) Perylene “BgP”	II	<b>0.96</b> (0.5 - 1)	~1 <b>0.32 - 1.00</b> 0.17 - ~1 0.98	-5.9 - 1.8 10 - 24 0 - 30 0 - 30	1 7 16(range) 16(median)
Dibenz (a,h) Anthracene “dBA”		<b>1</b> (0.98 - 1)	<b>0.29 - ~1</b> > 0.95	0 - 30 0 - 30	16(range) 16(median)
Indeno (1,2,3-c,d) Pyrene “IPyr”		<b>0.99</b> (0.9 - 1)	0.77 - 1.00 <b>0.46 - ~1</b> > 0.989	10 - 24 0 - 30 0 - 30	7 16(range) 16(median)
Dinitropyrenes “DNPs”	II	<b>0.4</b> (0.03 - 0.9)			
PAH's (as a group)	II				

**Table C.3.-(1). Vapor Particle Partitioning Summary  
for Compounds Considered in this Study**

Chemical or Group	Level	Estimated Fraction Adsorbed to Particle Phase in Atmosphere Based on Calculations in Appendix C [Central Estimate ( <b>bold</b> ) T = 290°K; Aerosol surface area = 3.5e-6 cm <sup>2</sup> /cm <sup>3</sup> ] [RANGE (in parentheses): 310 to 260 °K; 4.2e-7 to 1.1e-5 cm <sup>2</sup> /cm <sup>3</sup> ]	Examples from the Literature of Information Regarding Vapor/Particle Partitioning		
			fraction adsorbed to atmospheric particles	Temperature (°C)	Reference (see end of Table)
<b>References for above Table</b>					
(1) Kaupp and Umlauf, 1990 (Northern Bavaria, Germany: urban area)					
(2) Hawthorne et al., 1996 (South Dakota, U.S.: agricultural area)					
(3) Nakano et al., 1990a (Japan, urban area) (Note: The average particle-associated fraction was not explicitly reported; for the estimates of average particle-associated fraction reported in this table, the reported average particle-phase concentration was divided by reported average total particle- + vapor-phase concentration.)					
(4) Bidleman, Billings, and Foreman, 1986 (Columbia, South Carolina, U.S.; New Bedford, Mass., U.S.; Denver, Colorado, U.S.; Stockholm, Sweden: all urban areas). (Note: averages given here, as reported in paper, based on correlations of field data)					
(5) Kurokawa et al., 1996 (Japan: 2 urban sites, 1 rural site)					
(6) Nakano et al., 1990b (Kobe, Japan: urban area)					
(7) Baker and Eisenreich, 1990 (over Lake Superior)					
(8) Yamasaki et al., 1982 (Osaka City, Japan: urban area)					
(9) Albaiges et al., 1991 (Barcelona, Spain: urban area)					
(10) Gundel et al., 1995 (a: partitioning to simulated environmental tobacco smoke was studied; a relatively high aerosol concentration was employed; b: partitioning in laboratory air - denuder method; c: laboratory air - filter-sorbent (conventional) method)					
(11) Schroeder et al., 1991					
(12) Lamborg et al., 1994					
(13) Harrison and Laxen, 1978 (as cited in Grandjean and Nielsen, 1979)					
(14) information downloaded from U.S. National Institutes of Health <u>Hazardous Substances Database</u> (HSDB), Nov.- Dec., 1996					
(15) Eitzer and Hites, 1989a (Bloomington, Indiana, urban area)					
(16) Gustafson & Dickhut, 1997 (Southern Chesapeake Bay region; 4 sites: rural, semi-urban, urban, industrial)					

## Appendix C.4.

### Vapor-Particle Partitioning of PAH's: Detailed Comparison of Theoretical Estimates with Recent Experimental Data

In a recent paper, a detailed set of vapor/particle partitioning data for PAH's is described (Gustafson and Dickhut, 1997). The supplementary data (i.e., the detailed data set) was obtained and a comparison was made between the measurements and the "simplified" theoretical estimates used in this analysis.

The measurements were made at four sites in the southern Chesapeake Bay region, including one rural site, one semi-urban site, one urban site, and one industrial site (as characterized by the authors). Various measurements of the gas and particle phase concentrations of PAH's were made at the four sites, over the period from October 1993 through May 1995 (the period of measurements at the four sites varied). In all, a total of 44 paired sets of vapor and particle measurements were made, with 24 of these being made at the Haven Beach (rural) site. A set of 14 PAH's were measured, as listed in Table C.4.-(1), below.

<b>Table C.4.-(1). List of PAH Compounds</b>					
Chemical	Measured by Gustafson and Dickhut (1997)	Specifically Identified on IJC Target Compound List	ATSDR List of 17 PAH's	USEPA List of 16 PAH's	USEPA List of 7 PAH's
naphthalene	0	0	0	1	0
acenaphthene	0	0	1	1	0
acenaphthylene	0	0	1	1	0
fluorene	1	0	1	1	0
phenanthrene	1	1	1	1	0
anthracene	1	1	1	1	0
pyrene	1	0	1	1	0
fluoranthene	1	0	1	1	0
chrysene	1	0	1	1	1
benz [ a ] anthracene	1	1	1	1	1
benzo [ b ] fluoranthene	1	0	1	1	1
benzo [ j ] fluoranthene	0	0	1	0	0
benzo [ k ] fluoranthene	1	0	1	1	1
benzo [ a ] pyrene	1	1	1	1	1
benzo [ e ] pyrene	1	0	1	0	0
perylene	0	1	0	0	0
benzo [ g,h,i ] perylene	1	1	1	1	0
dibenz [a,h] anthracene	1	0	1	1	1
indeno [ 1,2,3-c,d ] pyrene	1	0	1	1	1
<b>total # in list --&gt;</b>	<b>14</b>	<b>6</b>	<b>17</b>	<b>16</b>	<b>7</b>

The complete data set is summarized in Table C.4.-(2) (page C-29) and given in Table C.4.-(3) (pages C-46 through C-54), below. In Table C.4.-(3), an "n.d." means "not detected"; "n.q." means "not quantified". These were assumed to be the meaning of the abbreviations used by the authors. An average detection limit of 0.30 pg/m<sup>3</sup> was reported, and, this value was used in the calculations shown. In these Tables, the "fraction associated with particles" is calculated from the available data.

When either the vapor or particle phase measurement was reported as "n.q.", or, if both the vapor and particle phase measurements were reported as "n.d.", then it was assumed that no estimate of the vapor/particle partitioning could be made from the data. In these cases, the term "n.a." (for "not available") was used in Table C.4.-(3). In general, out of the 44 measurements, about 40 estimates could be made for each of the PAH's measured.

A summary of the theoretical predictions for PAH's — as described in earlier portions of this Appendix — is shown in Figure C.4.-(1). In this Figure, the mid-range estimates are shown as "data points" and the low- and high-range of the estimates are shown as "error bars".

A comparison of the measurements of Dickhut and Gustafson (1997) with the simple theory used in this analysis is summarized in Table C.4.-(2). A plot of the median experimental measurements vs. the mid-range theoretical estimates is shown in Figure C.4.-(2). A detailed set of plots showing the experimental measurements and the theoretical predictions for each of the 14 PAH's measured are given as Figures C.4.-(3) through C.4.-(16).

It can be seen from the overall summary plot [Figure C.4.-(2)] that for most of the PAH's considered, the simple theory has done a relatively adequate job of predicting the overall tendency of the compounds. That is, compounds measured largely in the vapor phase were more or less predicted to exist largely in the vapor phase, etc.

For one (and maybe two) compounds, the predictions seem to be qualitatively wrong. Benzo(b)Fluoranthene is predicted by the theory to exist largely in the vapor phase. The particle-associated fractions are theoretically estimated to be:

low estimate	= 0.002
mid-range estimate	= 0.050
high-range estimate	= 0.520

There were 44 available measurements for benzo(b)fluoranthene; a statistical summary of the particle-associated fractions of these measurements is as follows:

minimum	= 0.21
maximum	= ~ 1
median	= 0.93

The reason for this discrepancy can not be unambiguously determined at this time, but, likely explanations are the following:

- The physical-chemical properties used for this compound were in error (i.e., the vapor-pressure may have been incorrect);
- Factors leading towards increased particle associated fractions (as discussed below) played a more dramatic role for this compound.

A similar but less dramatic discrepancy is seen for Benzo(a)Anthracene. In fact, the discrepancy was even larger than displayed, prompting a reconsideration of physical-chemical property data for this compound. A revised value for the vapor/pressure was adopted (as cited in Howard and Meylan, 1997), and the earlier used value (taken from MacKay et al, 1992) was discarded.

Even with this "correction" the theoretical predictions for Benzo(a)Anthracene indicate a lower particle associated fraction than observed. However, as shown in Figure C.4.-(8), there is somewhat of an overlap between the measured and theoretical ranges.

Throughout the many comparisons shown in this Appendix, there is a general pattern of the measured particle-associated fractions being somewhat higher than the predicted values. There are many possible reasons for this systematic trend, including the following:

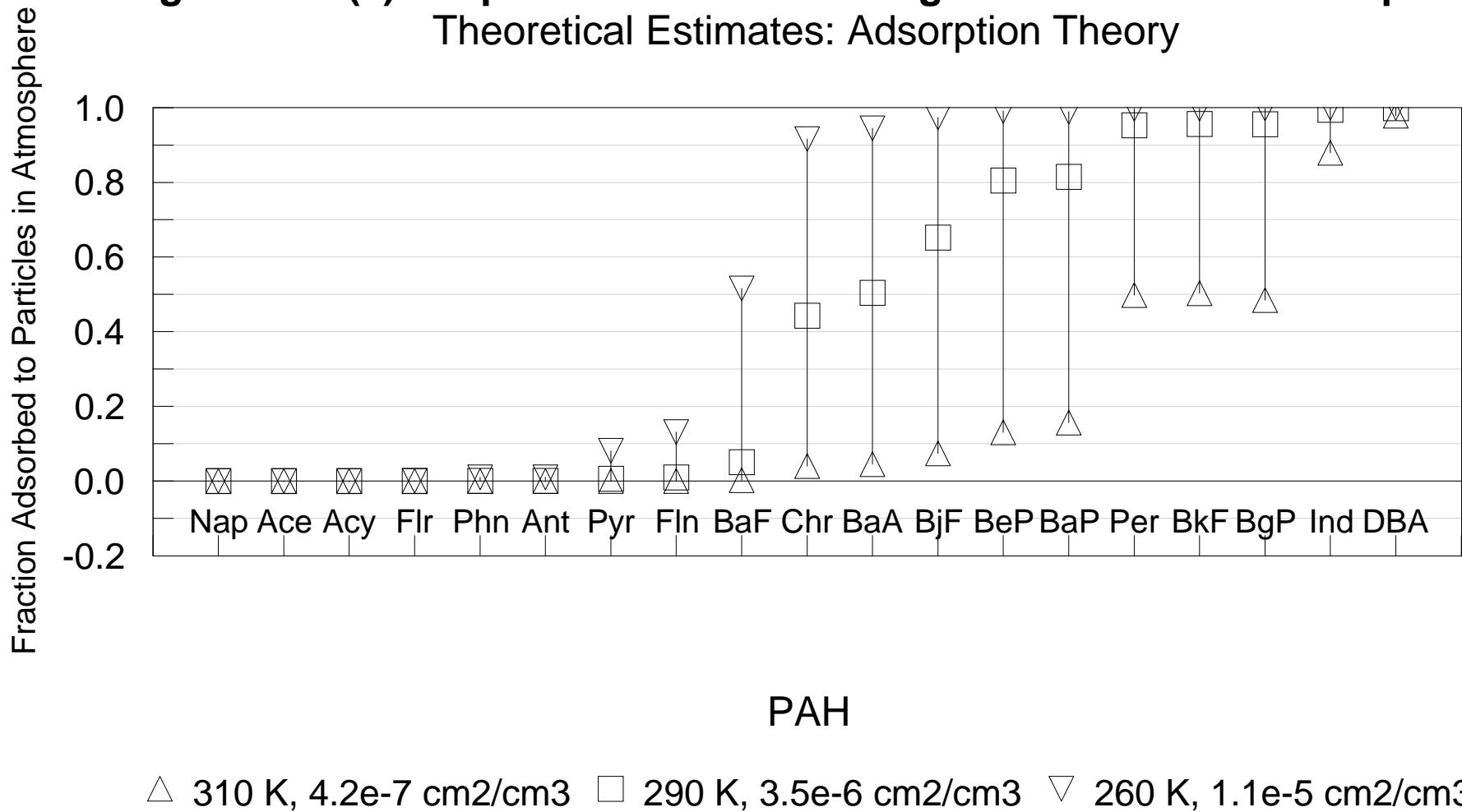
- The parameters used in the simplified absorption theory were not exactly appropriate for the PAH's and atmospheric conditions measured (i.e., there are potential "errors" in Junge's constant or the aerosol surface area, etc.);
- The physical-chemical properties for the PAH's are not exactly specified (i.e., there could have been errors in the "underlying data" used, or, possibly more likely, a systematic bias in the simplified extrapolation procedures used in this analysis could exist);
- An absorption theory or combined absorption/adsorption theory should have been used;
- A fraction of the PAH's are non-exchangeable;
- The measured particle-associated fractions are artificially high due to adsorption/absorption of gas-phase material onto particles already collected by the filter (a potential bias common to these types of measurements and acknowledged by the authors).

In reality, probably all of the above potential sources of error play a role in the differences observed between the measurements and the theoretical predictions.

**Table C.4-(2)****SUMMARY DATA from Gustafson and Dickhut, 1997: ES&T 31:140-147 (supplementary information)**

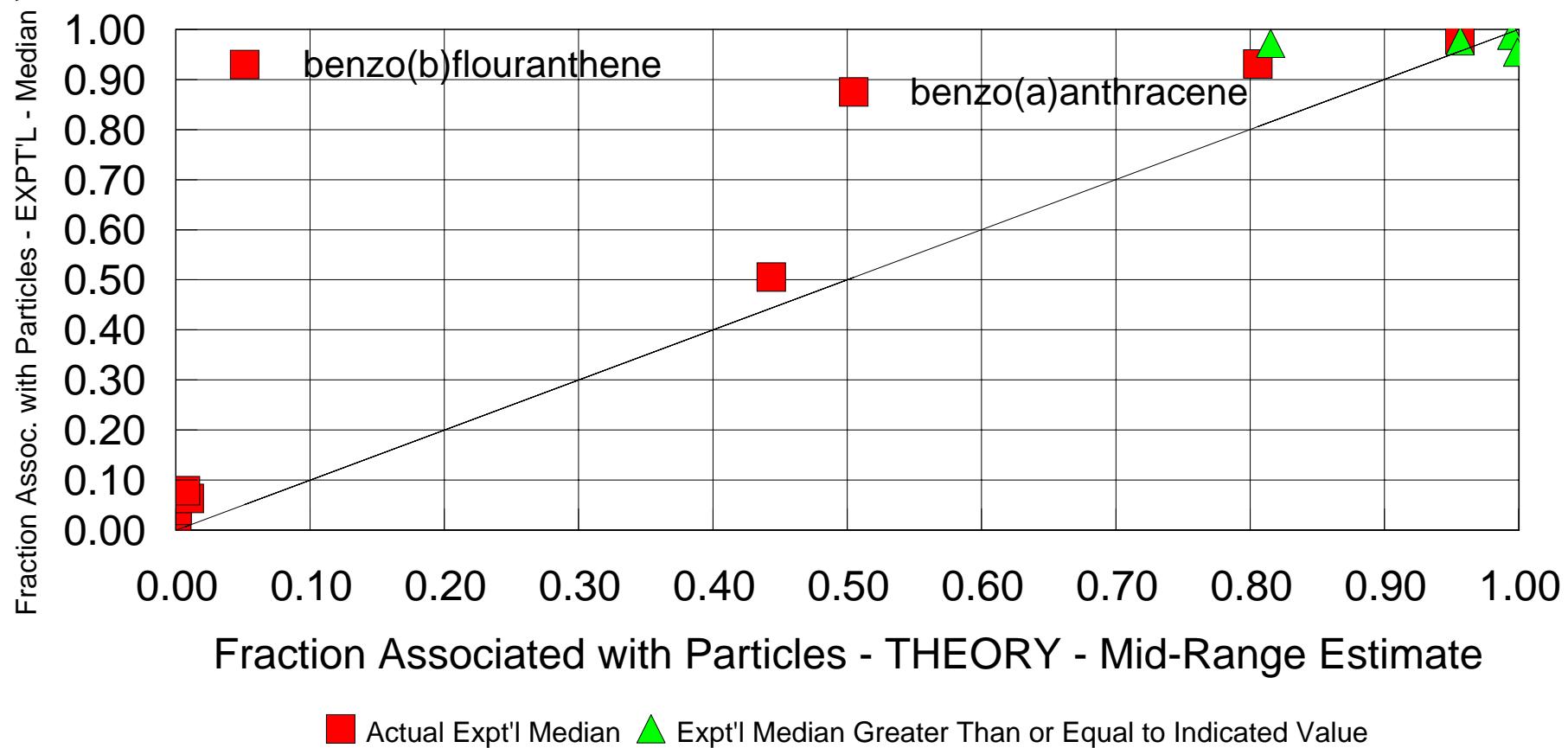
	TOTAL	TOTAL	TOTAL	TOTAL	TOTAL	TOTAL	TOTAL	TOTAL	TOTAL	THEORY	THEORY	THEORY			
	# of "Greater"	# of "Less"								Junge theory	Junge theory	Junge theory			
	Count	Thans"	Thans"		Min	Max	Median	Avg	Std	low-range	mid-range	high-range			
					fraction in particle phase										
fluorene	39	0	0		0.0004	0.0166	0.0039	0.0046	0.0035	0.0000	0.0001	0.0012			
phenanthrene	42	0	0		0.0004	0.1025	0.0103	0.0206	0.0249	0.0000	0.0008	0.0100			
anthracene	39	15	0		0.0006	>	0.9680	0.0400	>	0.3685	0.4407	0.0001	0.0010	0.0099	
fluoranthene	43	0	0		0.0014	0.4422	0.0636	0.1079	0.1126	0.0005	0.0099	0.1312			
pyrene	43	0	0		0.0050	0.5172	0.0795	0.1203	0.1336	0.0004	0.0070	0.0815			
benzo(a)anthracene	42	20	3		0.0161	>	0.9972	0.8753	>	0.7213	0.3258	0.0457	0.5048	0.9448	
chrysene	44	1	0		0.0118	>	0.9978	0.5058	>	0.5110	0.2903	0.0403	0.4432	0.9160	
benzo(b)flouranthene	44	3	0		0.2082	>	0.9990	0.9299	>	0.8304	0.1943	0.0023	0.0511	0.5159	
benzo(k)flouranthene	43	24	0		0.5030	>	0.9989	>	0.9769	>	0.9316	0.1116	0.5032	0.9564	0.9974
benzo(e)pyrene	44	6	0		0.1749	>	0.9987	0.9313	>	0.8154	0.2347	0.1309	0.8056	0.9910	
benzo(a)pyrene	43	25	0		0.0890	>	0.9983	>	0.9718	>	0.8663	0.2079	0.1564	0.8152	0.9891
indeno(123cd)pyrene	42	36	0		0.4637	>	0.9995	>	0.9881	>	0.9470	0.1149	0.8793	0.9948	0.9998
dibenzo(ah)anthracene	39	34	0		0.2940	>	0.9932	>	0.9544	>	0.8973	0.1333	0.9783	0.9990	0.9999
benzo(ghi)perylene	43	19	0		0.1709	>	0.9989	0.9796	>	0.8691	0.2073	0.4852	0.9561	0.9976	

**Figure C.4.-(1). Vapor/Particle Partitioning of PAH's in the Atmosphere**  
Theoretical Estimates: Adsorption Theory



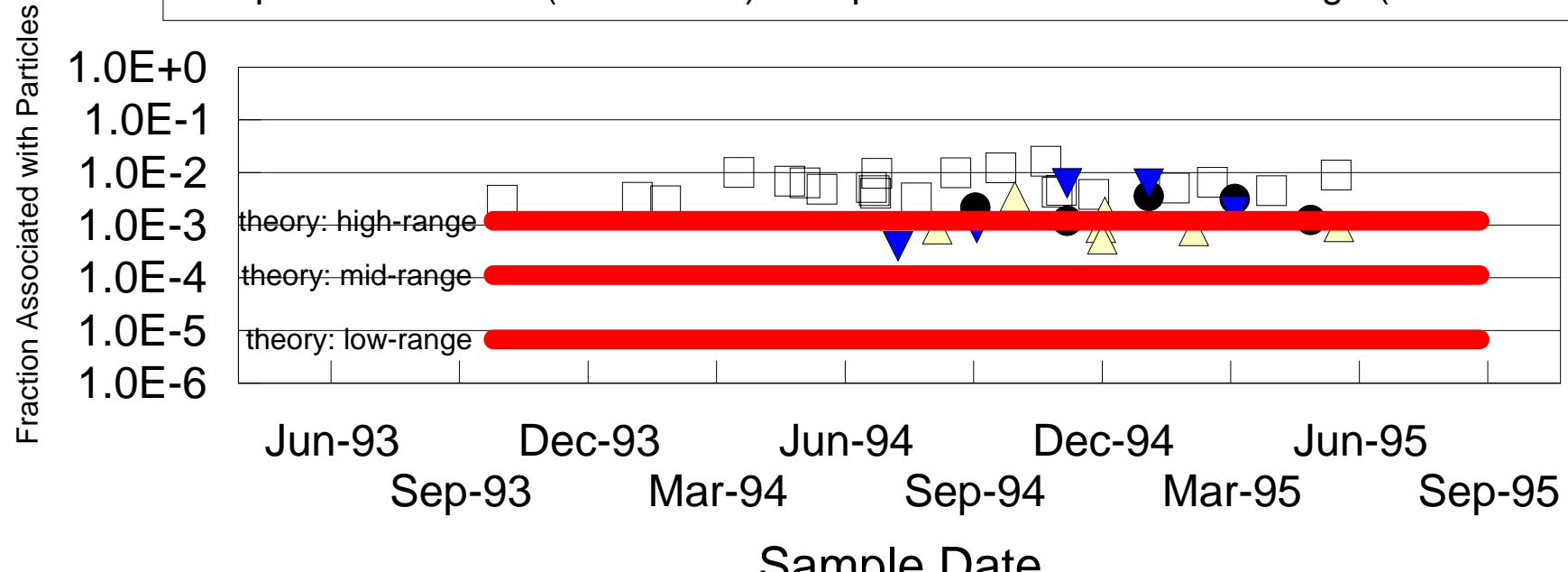
Estimates are based on Junge's Adsorption Theory, using subcooled liquid vapor pressure

**Figure C.4.-(2). Vapor/Particle Partitioning for PAH's (SUMMARY)**  
 Experimental Data (see note A) Compared with Theoretical Range (see note B)



A. Gustafson & Dickhut, ES&T 31:140-147, 1997. Atmos. meas. in the southern Ches. Bay region (~40 meas., 1993-1995)  
 B. Junge's Adsorption Theory, using subcooled liquid vapor pressure; Temp. = 290 K; Aerosol Surface Area = 3.5e-6 cm<sup>2</sup>/cm<sup>3</sup>

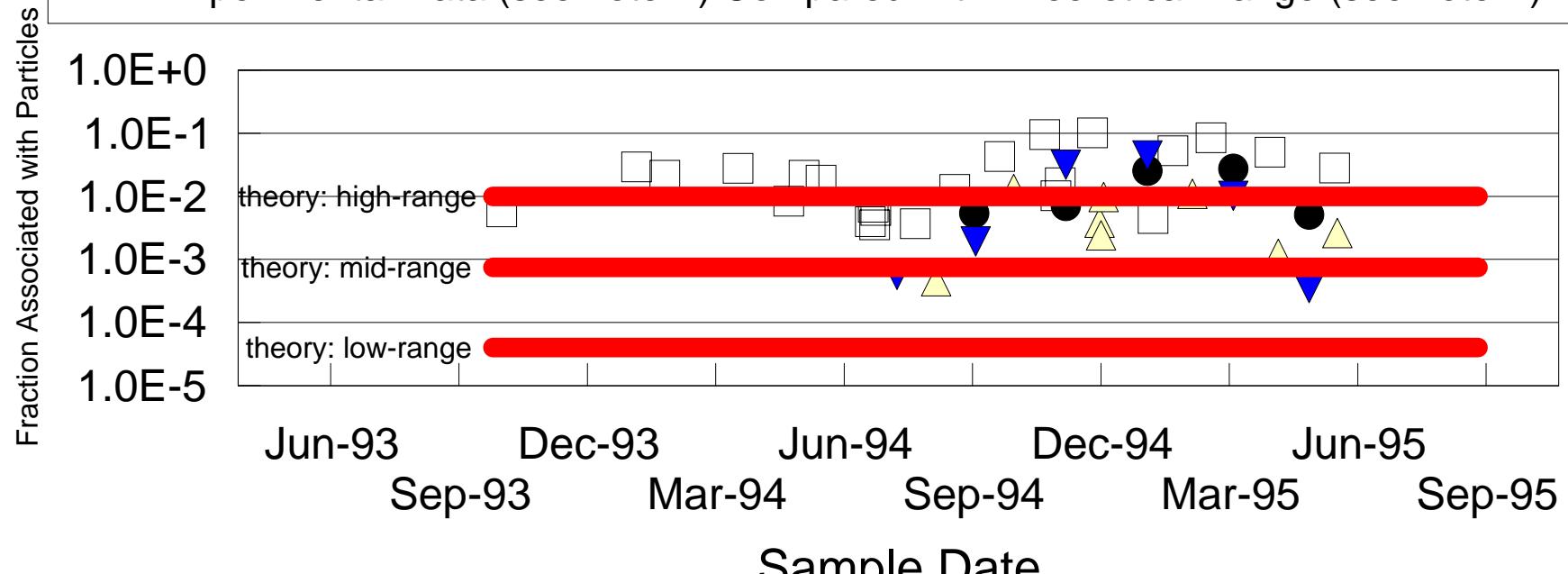
**Figure C.4.-(3). Vapor/Particle Partitioning for PAH's: FLOURENE**  
 Experimental Data (see note A) Compared with Theoretical Range (see note B)



□ Haven Beach (rural)	▼ Hampton (urban)
△ York River (semi-urban)	— Theory: Low-, Mid-, High-Range
● Elizabeth River (industrial)	

A: Gustafson & Dickhut, ES&T 31:140-147, 1997 (sample durations 4 - 10 hours)  
 B: Junge ads. (subcooled liq.Vp); Low:T=310K; Surface Area=4.2e-7cm<sup>2</sup>/cm<sup>3</sup>;  
 Mid:290K, Surface Area=3.5e-6cm<sup>2</sup>/cm<sup>3</sup>; High:260K, Surface Area=1.1e-5cm<sup>2</sup>/cm<sup>3</sup>

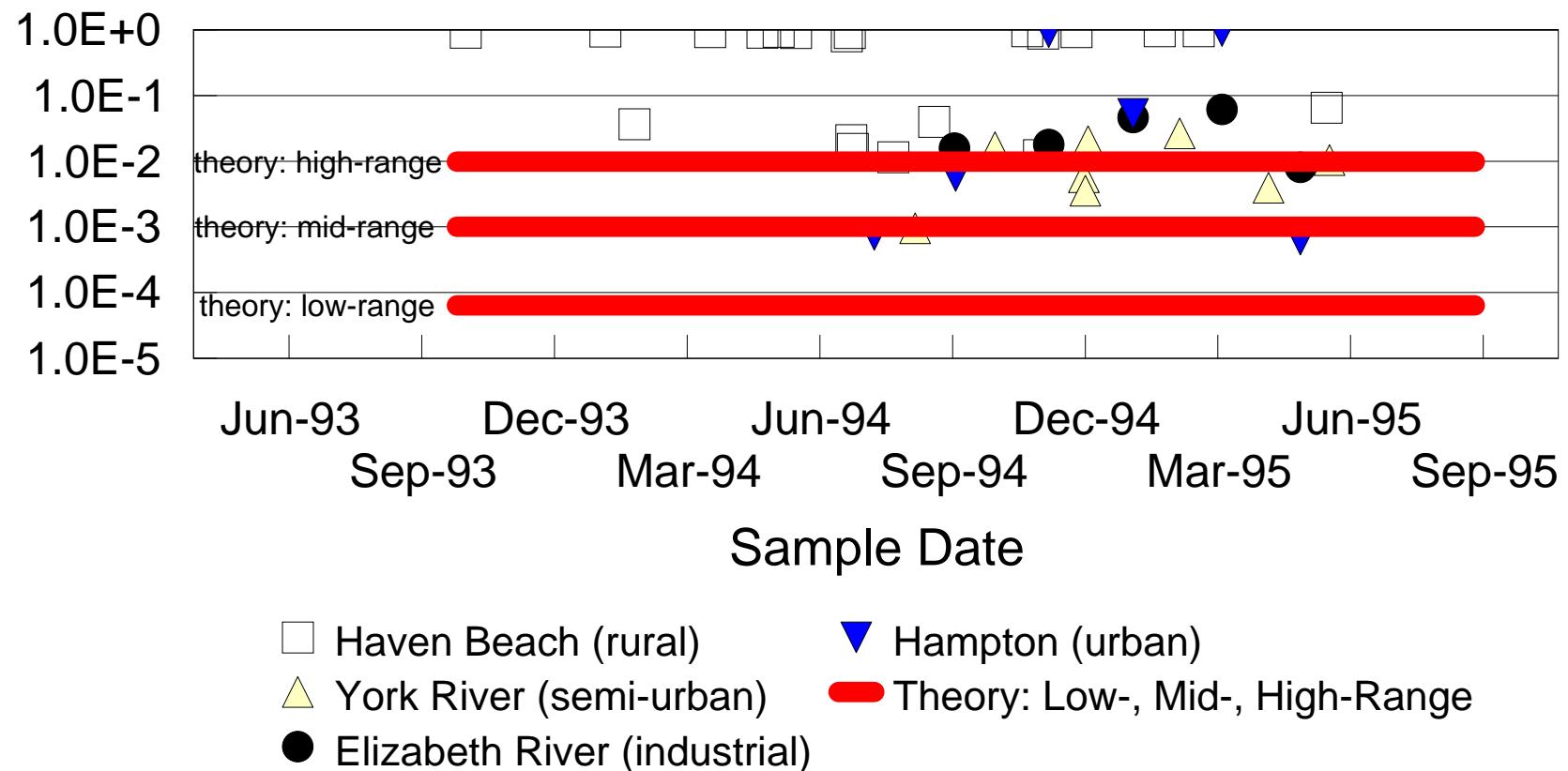
**Figure C.4.-(4). Vapor/Particle Partitioning for PAH's: PHENANTHRENE**  
 Experimental Data (see note A) Compared with Theoretical Range (see note B)



A: Gustafson & Dickhut, ES&T 31:140-147, 1997 (sample durations 4 - 10 hours)  
 B: Junge ads. (subcooled liq.Vp); Low:T=310K; Surface Area=4.2e-7cm<sup>2</sup>/cm<sup>3</sup>;  
 Mid:290K, Surface Area=3.5e-6cm<sup>2</sup>/cm<sup>3</sup>; High:260K, Surface Area=1.1e-5cm<sup>2</sup>/cm<sup>3</sup>

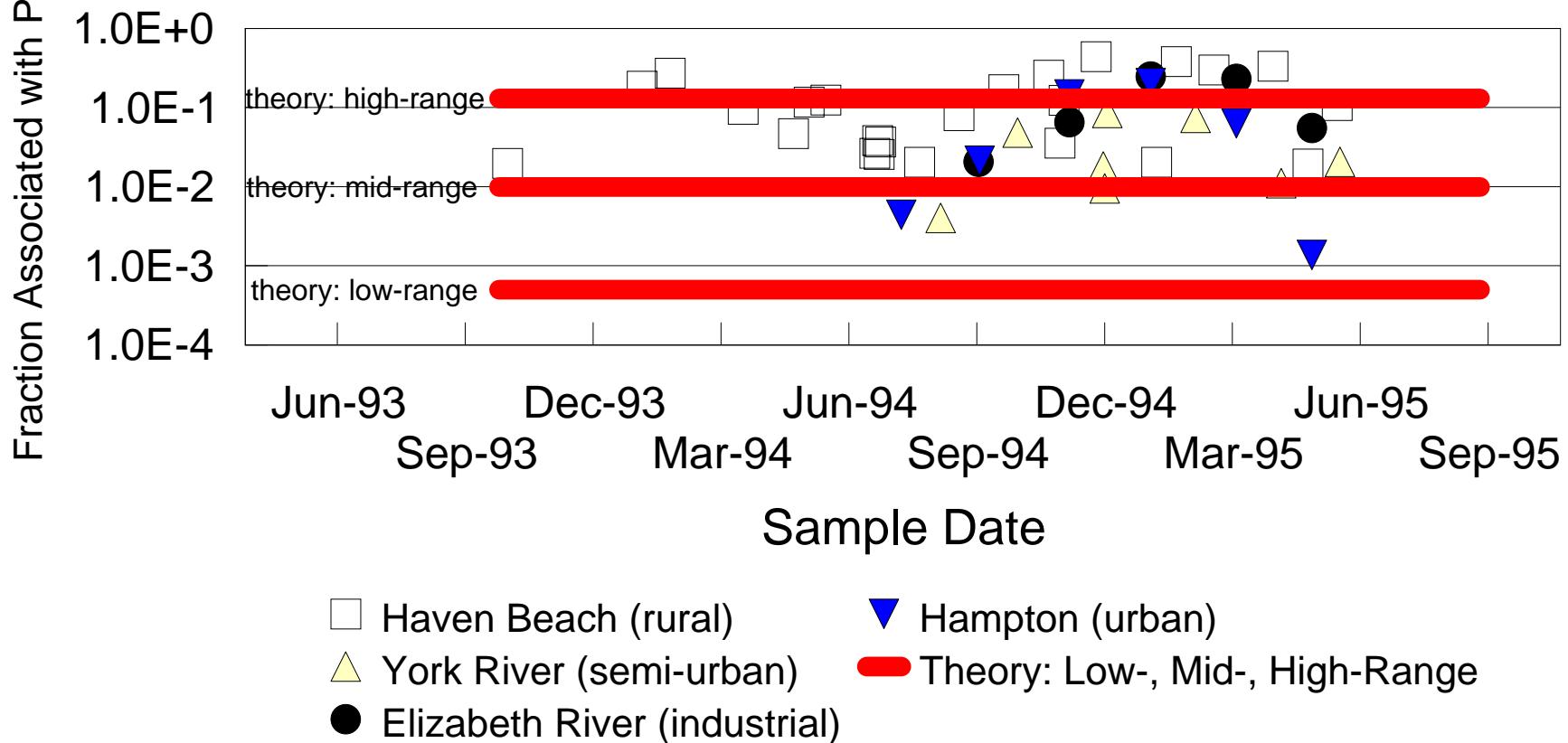
Fraction Associated with Particles

**Figure C.4.- (5). Vapor/Particle Partitioning for PAH's: ANTHRACENE**  
 Experimental Data (see note A) Compared with Theoretical Range (see note B)



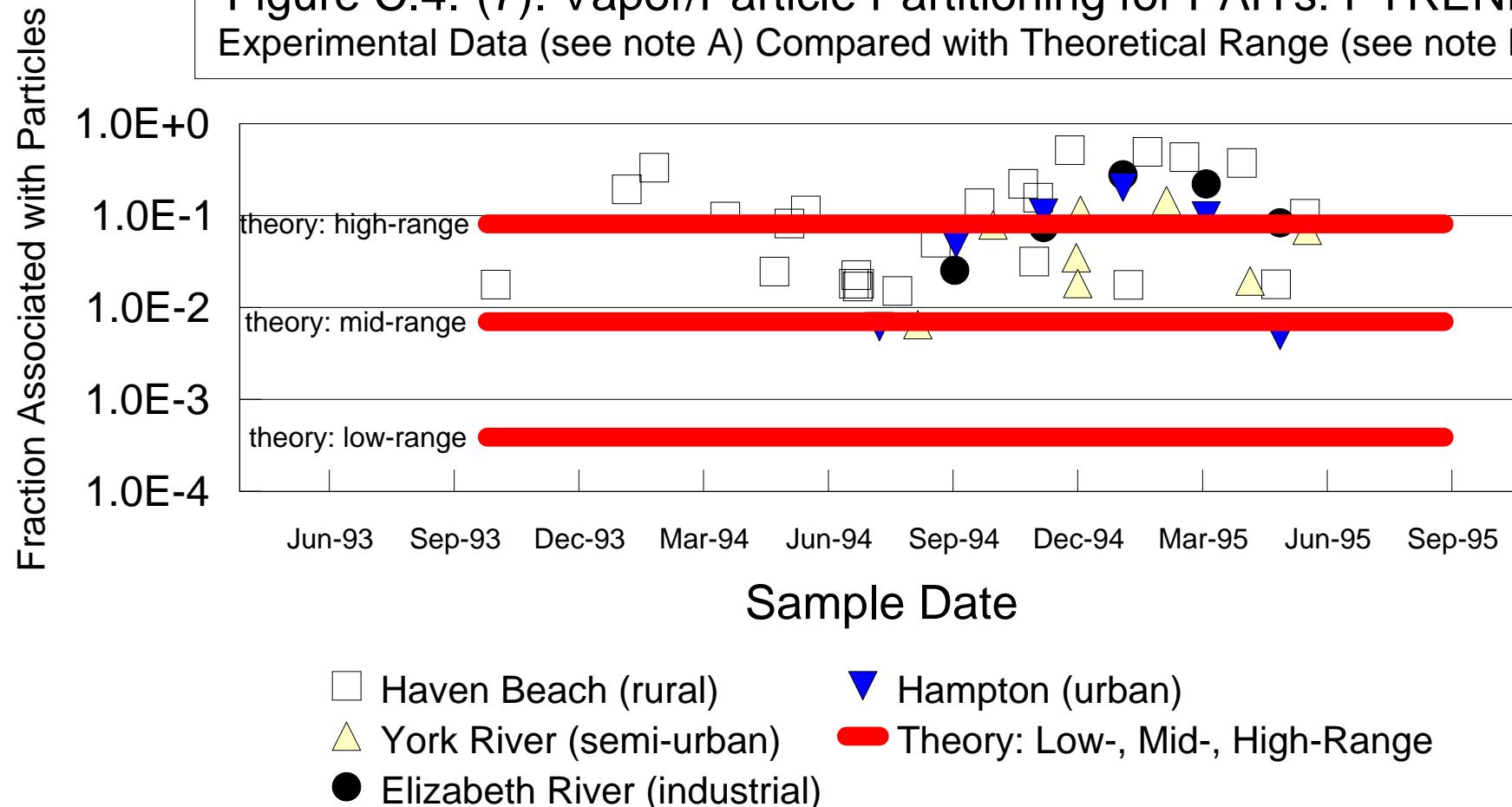
A: Gustafson & Dickhut, ES&T 31:140-147, 1997 (sample durations 4 - 10 hours)  
 B: Junge ads. (subcooled liq.Vp); Low:T=310K; Surface Area=4.2e-7cm<sup>2</sup>/cm<sup>3</sup>;  
 Mid:290K, Surface Area=3.5e-6cm<sup>2</sup>/cm<sup>3</sup>; High:260K, Surface Area=1.1e-5cm<sup>2</sup>/cm<sup>3</sup>

**Figure C.4.-(6). Vapor/Particle Partitioning for PAH's: FLUORANTHENE**  
 Experimental Data (see note A) Compared with Theoretical Range (see note B)



A: Gustafson & Dickhut, ES&T 31:140-147, 1997 (sample durations 4 - 10 hours)  
 B: Junge ads. (subcooled liq.Vp); Low:T=310K; Surface Area= $4.2e-7\text{cm}^2/\text{cm}^3$ ;  
 Mid:290K, Surface Area= $3.5e-6\text{cm}^2/\text{cm}^3$ ; High:260K, Surface Area= $1.1e-5\text{cm}^2/\text{cm}^3$

**Figure C.4.-(7). Vapor/Particle Partitioning for PAH's: PYRENE**  
 Experimental Data (see note A) Compared with Theoretical Range (see note B)



A: Gustafson & Dickhut, ES&T 31:140-147, 1997 (sample durations 4 - 10 hours)  
 B: Junge ads. (subcooled liq.Vp); Low:T=310K; Surface Area=4.2e-7cm<sup>2</sup>/cm<sup>3</sup>;  
 Mid:290K, Surface Area=3.5e-6cm<sup>2</sup>/cm<sup>3</sup>; High:260K, Surface Area=1.1e-5cm<sup>2</sup>/cm<sup>3</sup>

Figure C.4.-(8). Vapor/Particle Partitioning for PAH's: BENZO(a)ANTHRACENE  
Experimental Data (see note A) Compared with Theoretical Range (see note B)

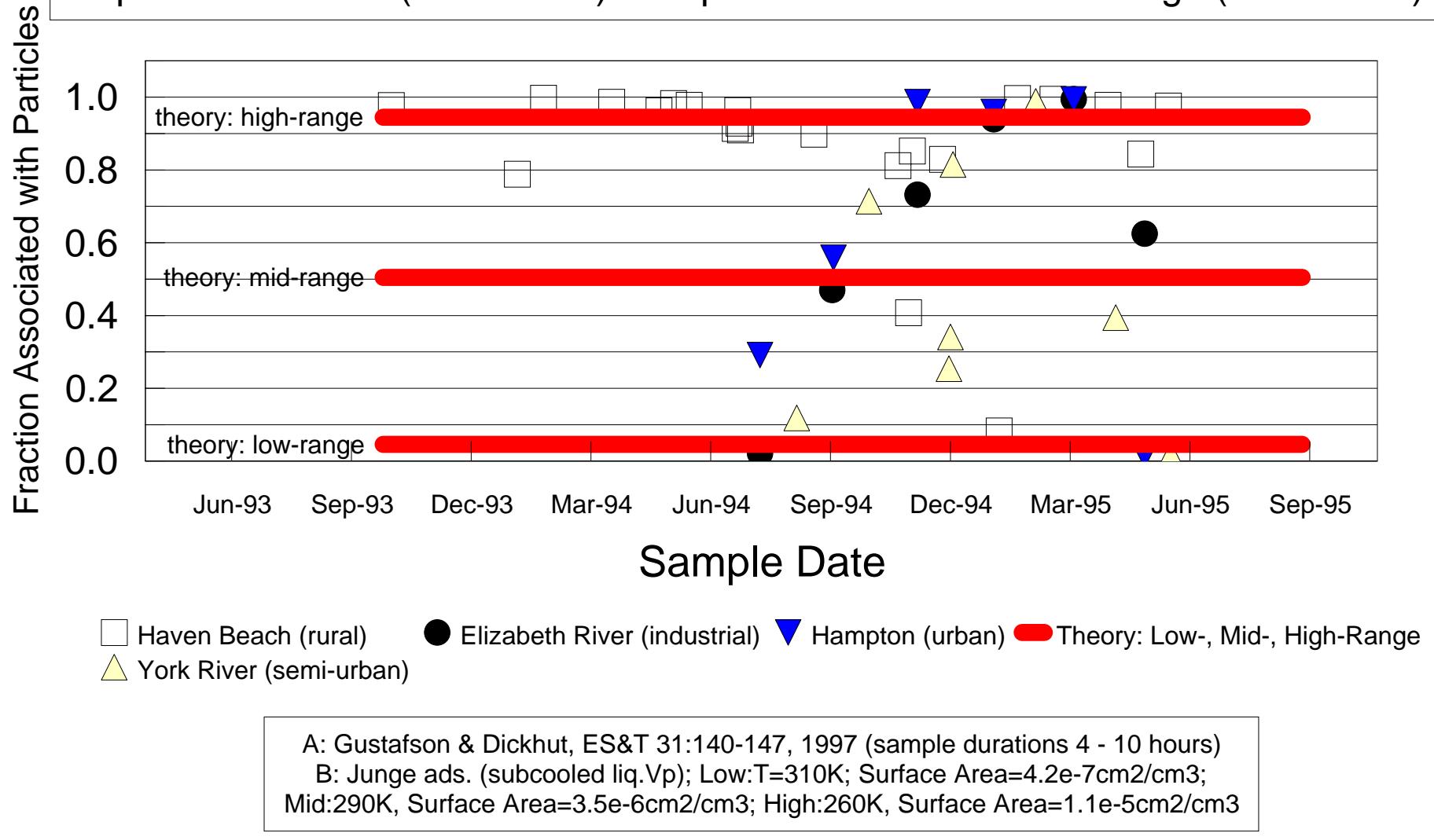


Figure C.4.-(9). Vapor/Particle Partitioning for PAH's: CHRYSENE  
Experimental Data (see note A) Compared with Theoretical Range (see note B)

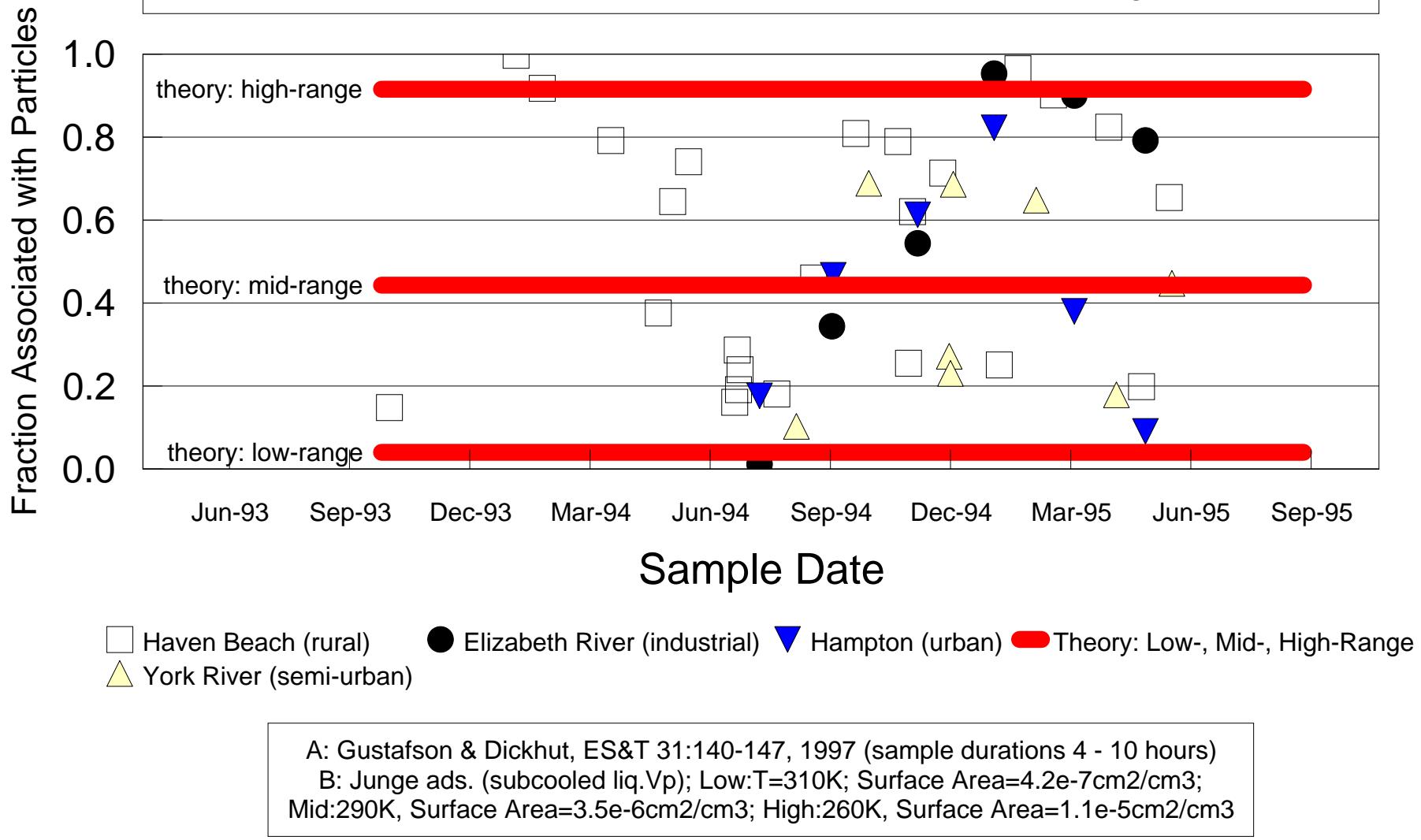


Figure C.4.-(10). Vapor/Particle Partitioning for PAH's: BENZO(b)FLUORANTHENE  
Experimental Data (see note A) Compared with Theoretical Range (see note B)

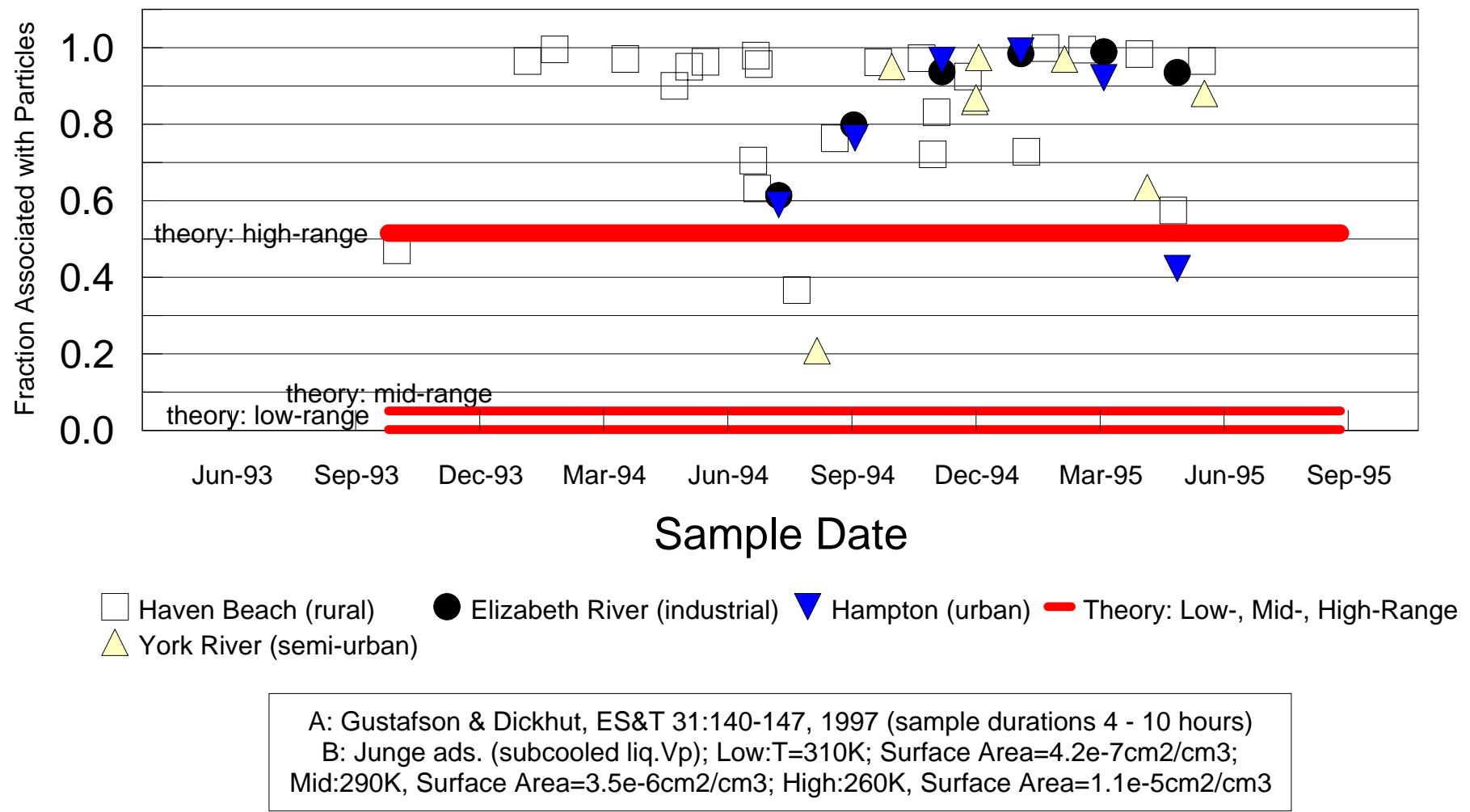
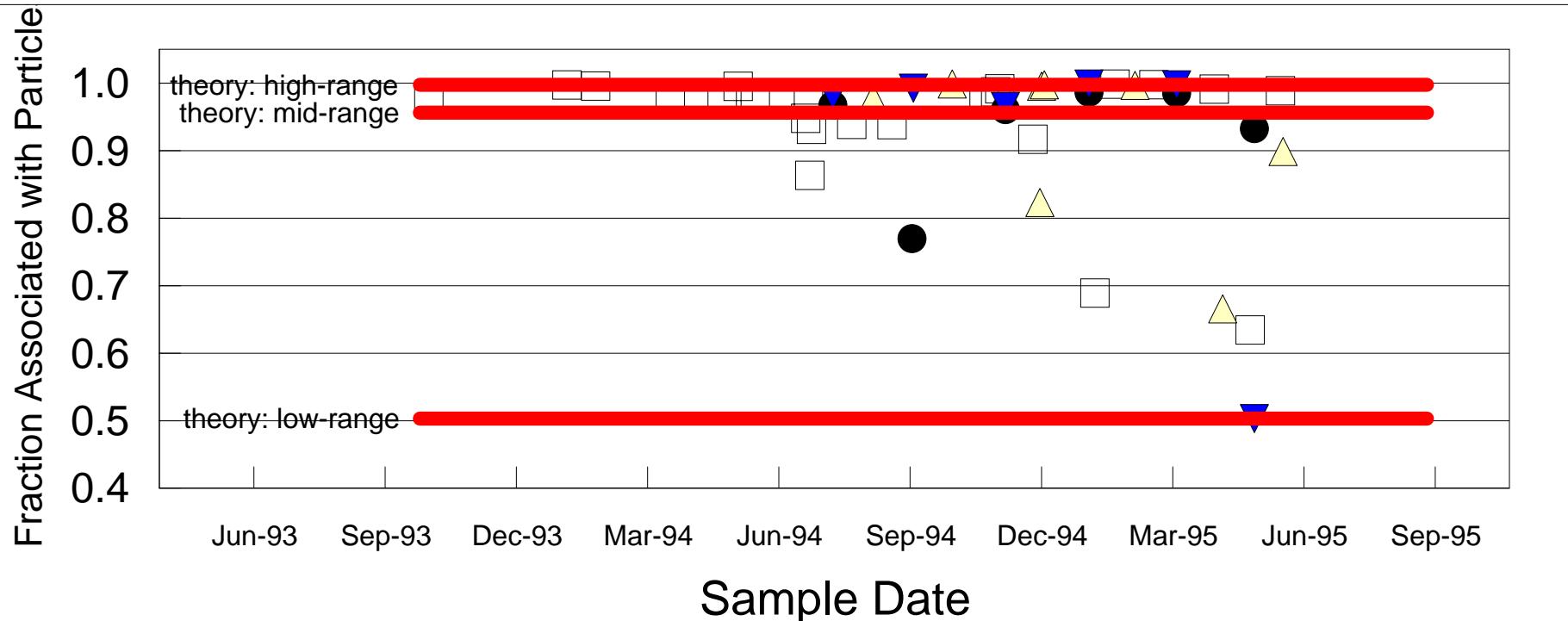


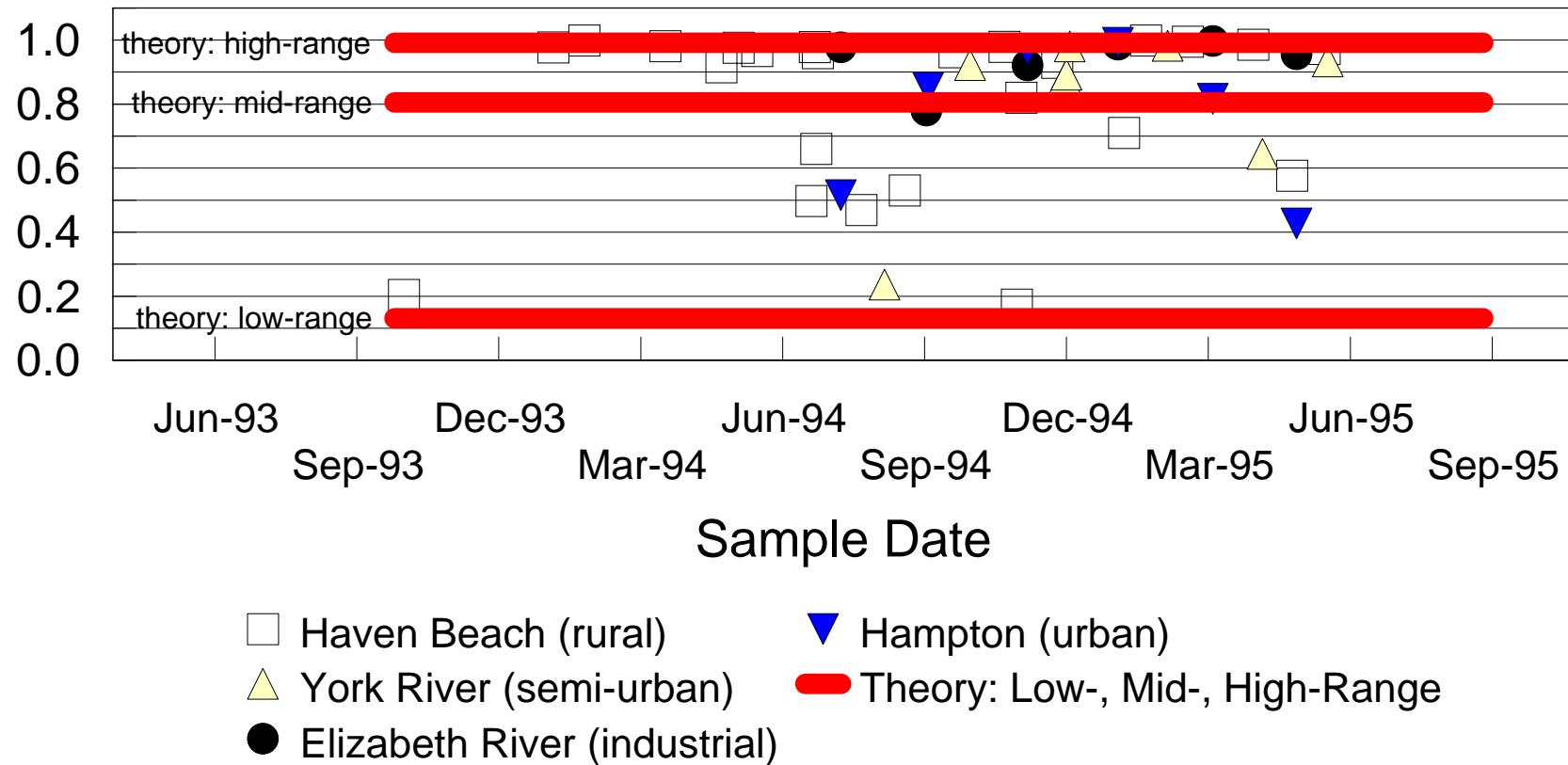
Figure C.4.-(11). Vapor/Particle Partitioning for PAH's: BENZO(k)FLUORANTHENE  
Experimental Data (see note A) Compared with Theoretical Range (see note B)



A: Gustafson & Dickhut, ES&T 31:140-147, 1997 (sample durations 4 - 10 hours)  
B: Junge ads. (subcooled liq.Vp); Low:T=310K; Surface Area=4.2e-7cm<sup>2</sup>/cm<sup>3</sup>;  
Mid:290K, Surface Area=3.5e-6cm<sup>2</sup>/cm<sup>3</sup>; High:260K, Surface Area=1.1e-5cm<sup>2</sup>/cm<sup>3</sup>

Fraction Associated with Particles

Figure C.4.-(12). Vapor/Particle Partitioning for PAH's: BENZO(e)PYRENE  
Experimental Data (see note A) Compared with Theoretical Range (see note B)

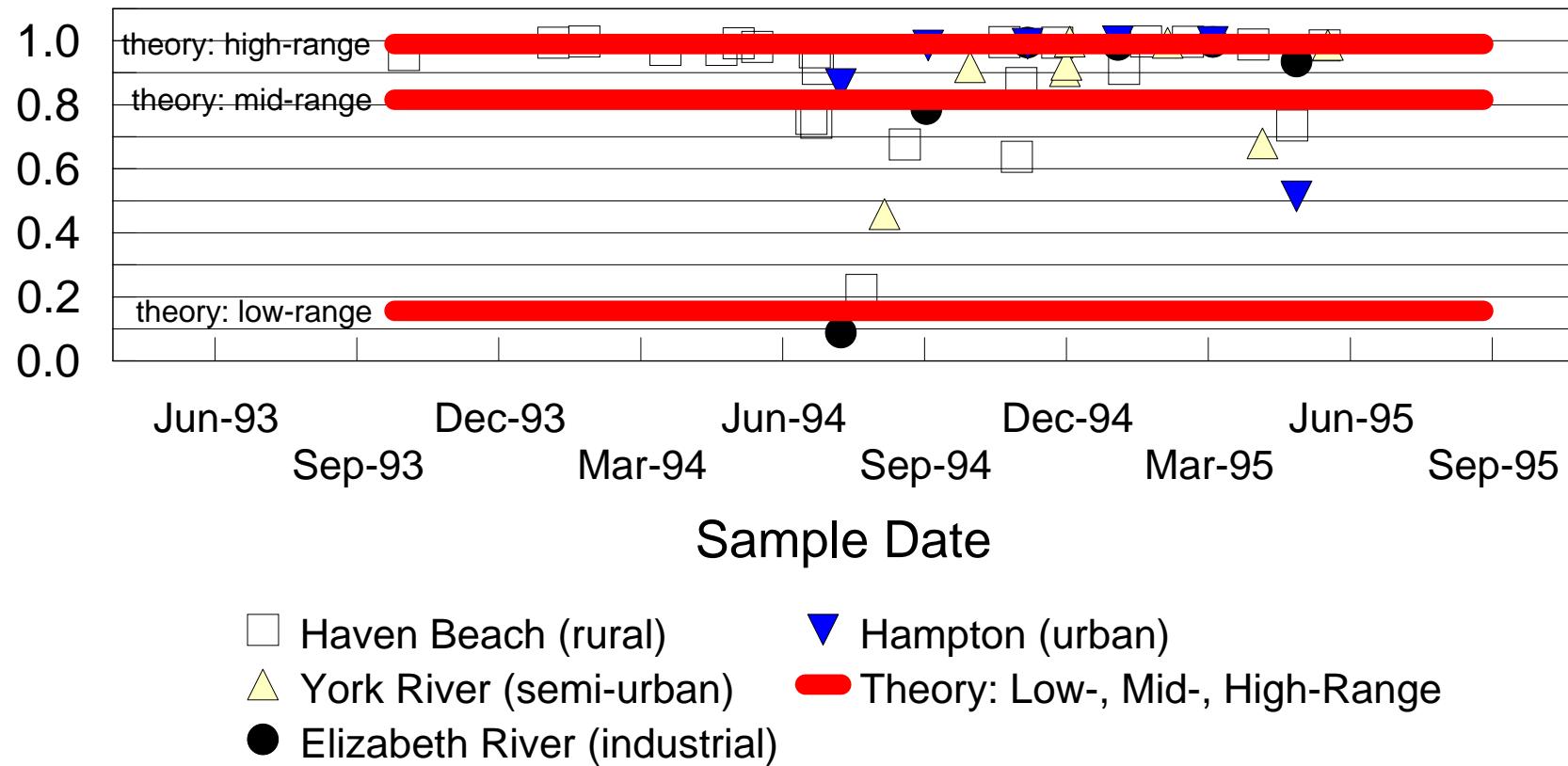


A: Gustafson & Dickhut, ES&T 31:140-147, 1997 (sample durations 4 - 10 hours)

B: Junge ads. (subcooled liq.Vp); Low:T=310K; Surface Area=4.2e-7cm<sup>2</sup>/cm<sup>3</sup>;  
Mid:290K, Surface Area=3.5e-6cm<sup>2</sup>/cm<sup>3</sup>; High:260K, Surface Area=1.1e-5cm<sup>2</sup>/cm<sup>3</sup>

Fraction Associated with Particles

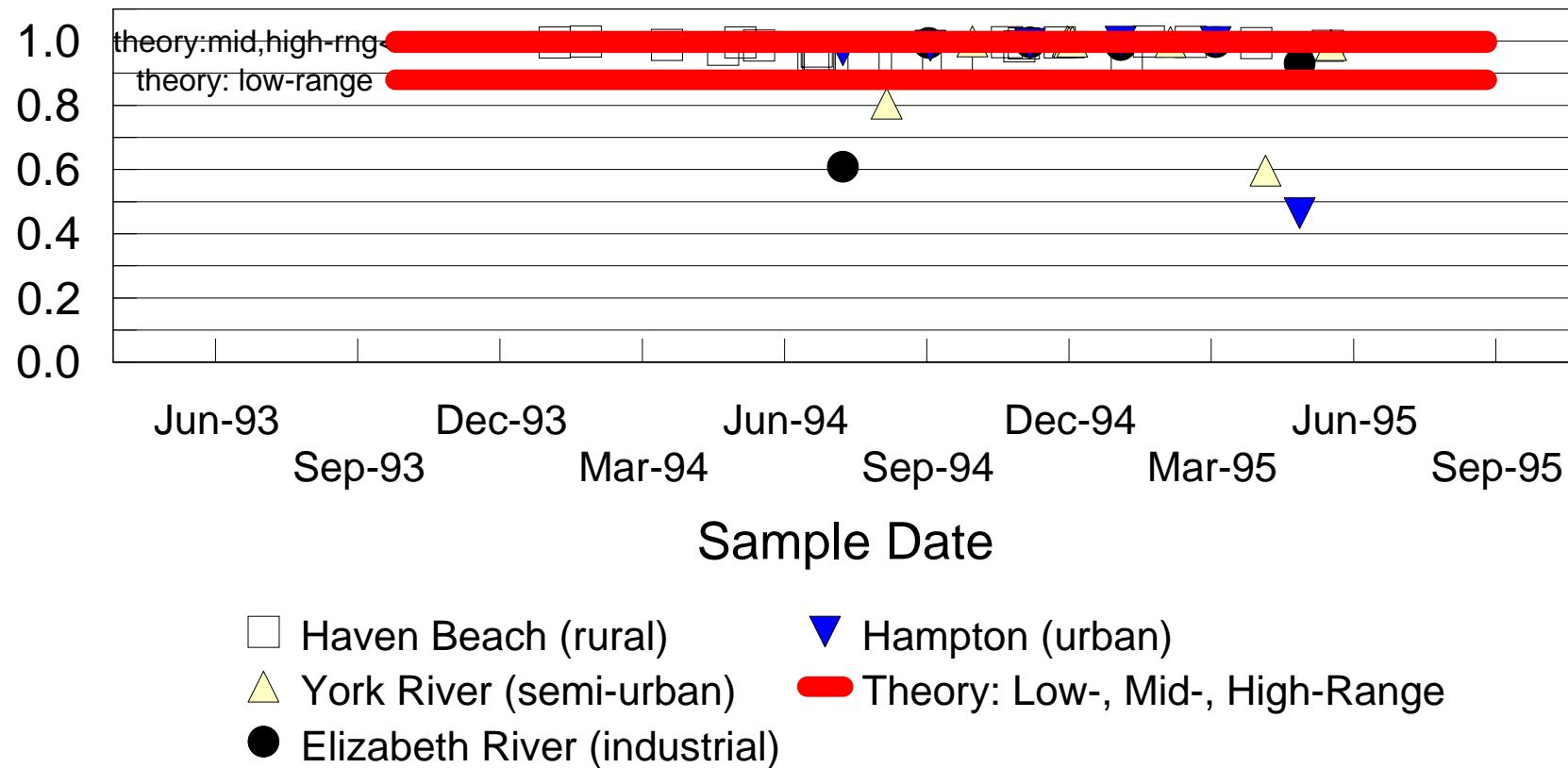
Figure C.4.-(13). Vapor/Particle Partitioning for PAH's: BENZO(a)PYRENE  
Experimental Data (see note A) Compared with Theoretical Range (see note B)



A: Gustafson & Dickhut, ES&T 31:140-147, 1997 (sample durations 4 - 10 hours)  
B: Junge ads. (subcooled liq.Vp); Low:T=310K; Surface Area=4.2e-7cm<sup>2</sup>/cm<sup>3</sup>;  
Mid:290K, Surface Area=3.5e-6cm<sup>2</sup>/cm<sup>3</sup>; High:260K, Surface Area=1.1e-5cm<sup>2</sup>/cm<sup>3</sup>

Fraction Associated with Particles

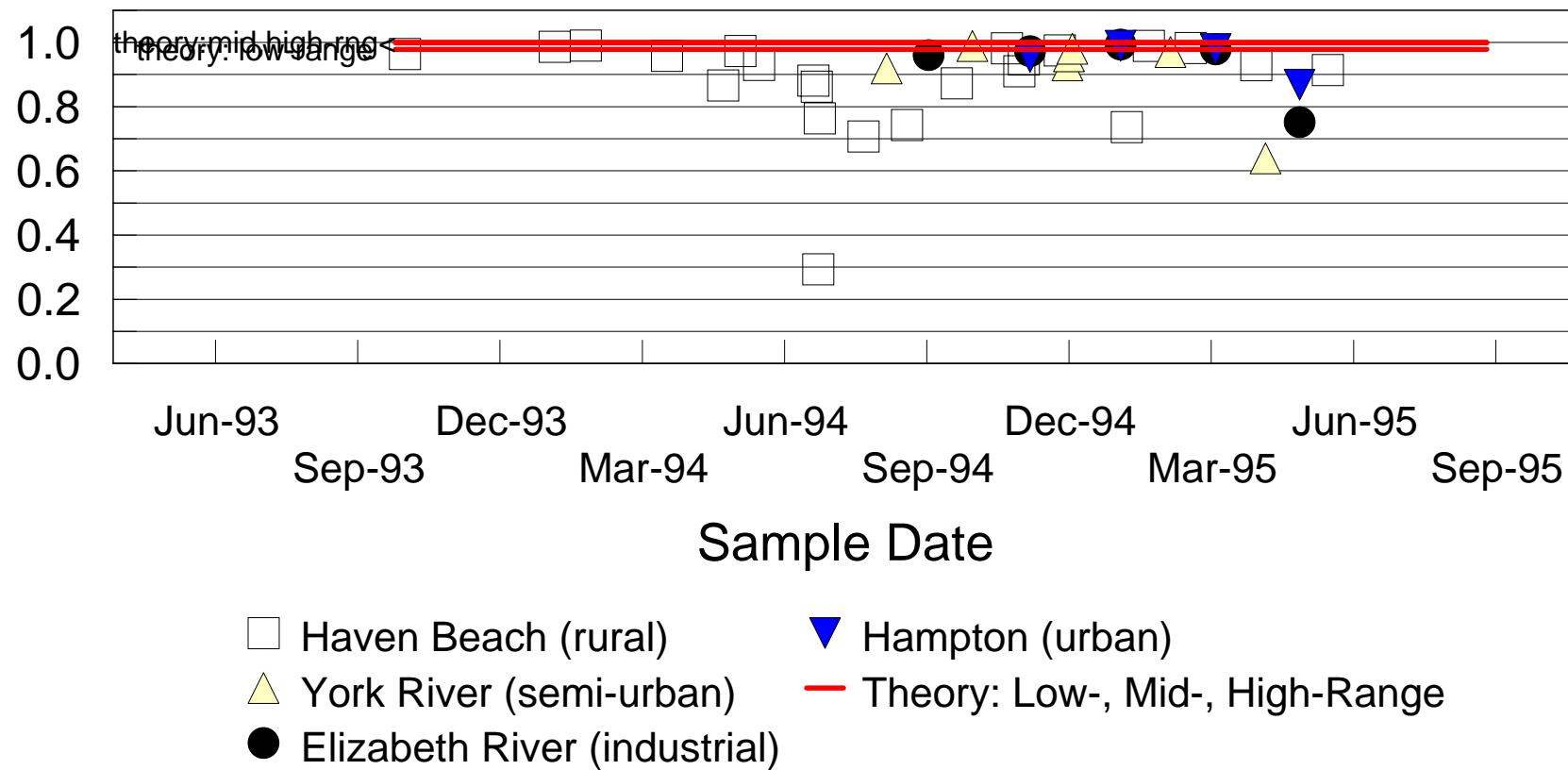
Figure C.4.-(14). Vapor/Particle Partitioning for PAH's: INDENO(1,2,3-cd)PYRENE  
Experimental Data (see note A) Compared with Theoretical Range (see note B)



A: Gustafson & Dickhut, ES&T 31:140-147, 1997 (sample durations 4 - 10 hours)  
B: Junge ads. (subcooled liq.Vp); Low:T=310K; Surface Area=4.2e-7cm<sup>2</sup>/cm<sup>3</sup>;  
Mid:290K, Surface Area=3.5e-6cm<sup>2</sup>/cm<sup>3</sup>; High:260K, Surface Area=1.1e-5cm<sup>2</sup>/cm<sup>3</sup>

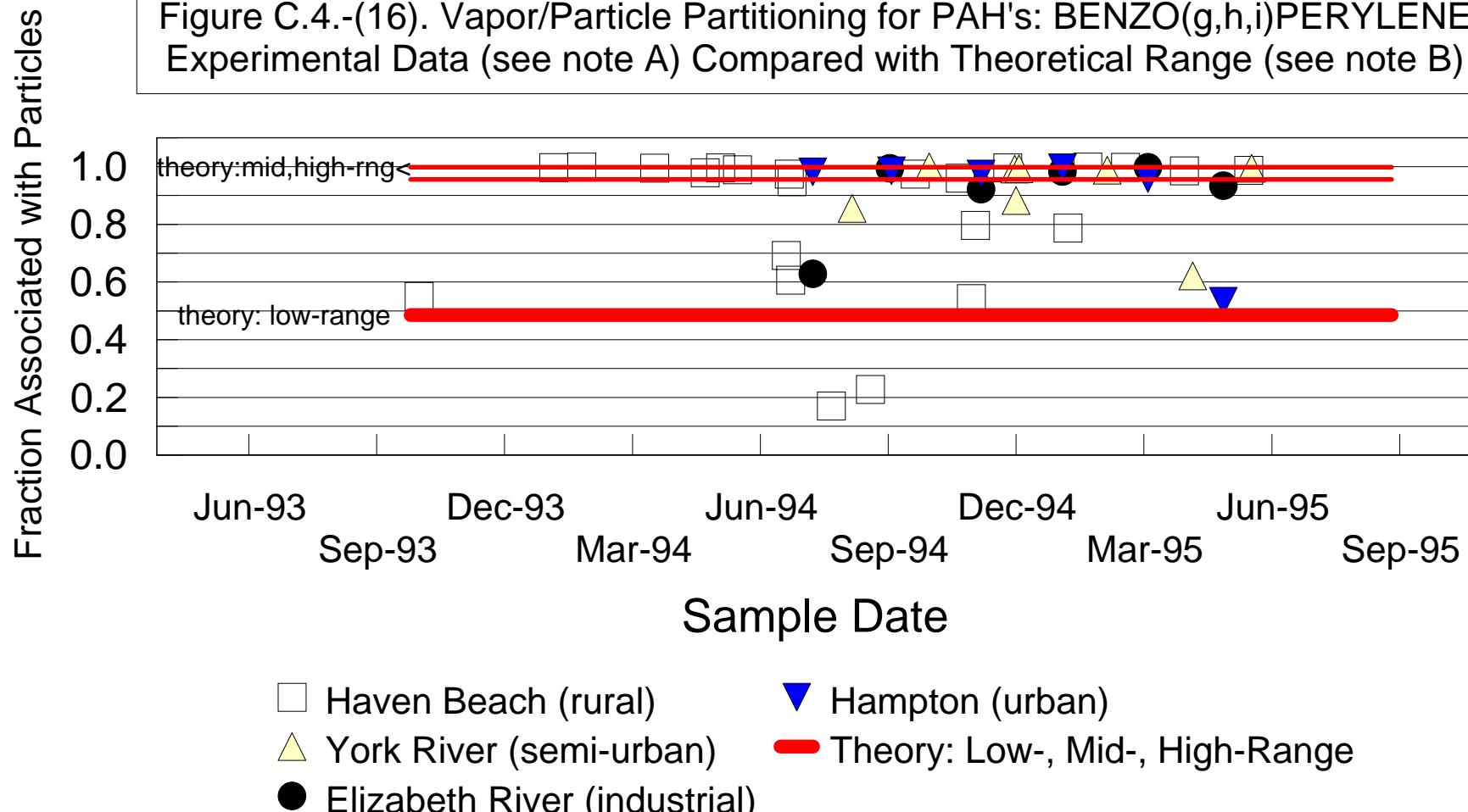
Fraction Associated with Particles

Figure C.4.-(15). Vapor/Particle Partitioning for PAH's: DIBENZO(a,h)ANTHRACENE  
Experimental Data (see note A) Compared with Theoretical Range (see note B)



A: Gustafson & Dickhut, ES&T 31:140-147, 1997 (sample durations 4 - 10 hours)  
B: Junge ads. (subcooled liq.Vp); Low:T=310K; Surface Area=4.2e-7cm<sup>2</sup>/cm<sup>3</sup>;  
Mid:290K, Surface Area=3.5e-6cm<sup>2</sup>/cm<sup>3</sup>; High:260K, Surface Area=1.1e-5cm<sup>2</sup>/cm<sup>3</sup>

Figure C.4.-(16). Vapor/Particle Partitioning for PAH's: BENZO(g,h,i)PERYLENE  
 Experimental Data (see note A) Compared with Theoretical Range (see note B)



A: Gustafson & Dickhut, ES&T 31:140-147, 1997 (sample durations 4 - 10 hours)  
 B: Junge ads. (subcooled liq.Vp); Low:T=310K; Surface Area=4.2e-7cm<sup>2</sup>/cm<sup>3</sup>;  
 Mid:290K, Surface Area=3.5e-6cm<sup>2</sup>/cm<sup>3</sup>; High:260K, Surface Area=1.1e-5cm<sup>2</sup>/cm<sup>3</sup>

Table C.4.(3)

## Data from Gustafson and Dickhut (1997)

(supplementary information)

value to use for ND =	HAVEN	HAVEN	HAVEN	HAVEN	HAVEN	HAVEN	HAVEN			
<b>0.3</b>	BEACH	BEACH	BEACH	BEACH	BEACH	BEACH	BEACH			
pg/m <sup>3</sup> (avg value per article)	07-Oct-93	11-Jan-94	31-Jan-94	24-Mar-94	29-Apr-94					
	det- pg/m <sup>3</sup>	det- pg/m <sup>3</sup>	det- pg/m <sup>3</sup>	det- pg/m <sup>3</sup>	det- pg/m <sup>3</sup>	det- pg/m <sup>3</sup>	det- pg/m <sup>3</sup>			
	ect? gas phase	ect? gas phase	ect? gas phase	ect? gas phase	ect? gas phase	ect? gas phase	ect? gas phase			
fluorene	1	2398.91	1	2446.07	1	3052.15	1	663.91	1	482.43
phenanthrene	1	5617.75	1	3579.03	1	6900.56	1	1729.54	1	3395.83
anthracene	0	<b>0.30</b>	0	<b>0.30</b>	1	292.84	0	<b>0.30</b>	0	<b>0.30</b>
fluoranthene	1	651.16	1	588.62	1	599.5	1	354.95	1	535.75
pyrene	1	942.49	1	449.17	1	396.3	1	339.36	1	967.82
benzo(a)anthracene	0	<b>0.30</b>	1	10.64	0	<b>0.30</b>	0	<b>0.30</b>	0	<b>0.30</b>
chrysene	1	74.04	0	<b>0.30</b>	1	22.9	1	22.77	1	32.85
benzo(b)flouranthene	1	17.18	1	4.24	1	1.2	1	2.2	1	2.13
benzo(k)flouranthene	0	<b>0.30</b>	0	<b>0.30</b>	1	1	1	1.16	0	<b>0.30</b>
benzo(e)pyrene	1	40.57	1	2.46	0	<b>0.30</b>	1	1.34	1	1.53
benzo(a)pyrene	0	<b>0.30</b>	0	<b>0.30</b>	0	<b>0.30</b>	1	0.61	0	<b>0.30</b>
indeno(123cd)pyrene	0	<b>0.30</b>	0	<b>0.30</b>	0	<b>0.30</b>	0	<b>0.30</b>	0	<b>0.30</b>
dibenzo(ah)anthracene	0	<b>0.30</b>	0	<b>0.30</b>	0	<b>0.30</b>	0	<b>0.30</b>	0	<b>0.30</b>
benzo(ghi)perylene	1	10.20	0	<b>0.30</b>	0	<b>0.30</b>	0	<b>0.30</b>	0	<b>0.30</b>
///	///	///	///	///	///	///	///	///	///	///
	det- pg/m <sup>3</sup>	det- pg/m <sup>3</sup>	det- pg/m <sup>3</sup>	det- pg/m <sup>3</sup>	det- pg/m <sup>3</sup>	det- pg/m <sup>3</sup>	det- pg/m <sup>3</sup>			
	ect? particle phase	ect? particle phase	ect? particle phase	ect? particle phase	ect? particle phase	ect? particle phase	ect? particle phase			
fluorene	1	7.279	1	8.361	1	8.990	1	6.807	1	3.358
phenanthrene	1	32.437	1	108.962	1	154.465	1	50.010	1	28.969
anthracene	1	3.089	1	6.593	1	11.264	1	4.416	1	3.121
fluoranthene	1	13.244	1	136.943	1	227.957	1	37.798	1	26.550
pyrene	1	17.210	1	108.713	1	199.634	1	37.086	1	24.577
benzo(a)anthracene	1	12.815	1	39.680	1	108.298	1	21.455	1	7.818
chrysene	1	12.946	1	138.436	1	258.172	1	86.925	1	19.842
benzo(b)flouranthene	1	15.293	1	118.607	1	282.670	1	72.587	1	19.305
benzo(k)flouranthene	1	10.571	1	122.957	1	252.678	1	45.599	1	13.927
benzo(e)pyrene	1	10.413	1	106.646	1	229.789	1	69.987	1	16.523
benzo(a)pyrene	1	6.477	1	48.973	1	170.597	1	21.270	1	10.353
indeno(123cd)pyrene	0	<b>0.300</b>	1	85.299	1	205.855	1	25.445	1	11.243
dibenzo(ah)anthracene	1	8.099	1	21.744	1	31.646	1	6.850	1	1.942
benzo(ghi)perylene	1	12.488	1	97.422	1	223.031	1	65.399	1	14.442
///	///	///	///	///	///	///	///	///	///	///
	fraction in particle phase		fraction in particle phase		fraction in particle phase		fraction in particle phase		fraction in particle phase	
fluorene	=	0.00303	=	0.00341	=	0.00294	=	0.01015	=	0.00691
phenanthrene	=	0.00574	=	0.02955	=	0.02189	=	0.02810	=	0.00846
anthracene	>	0.91148	>	0.95648	=	0.03704	>	0.93639	>	0.91231
fluoranthene	=	0.01993	=	0.18874	=	0.27549	=	0.09624	=	0.04722
pyrene	=	0.01793	=	0.19487	=	0.33499	=	0.09852	=	0.02477
benzo(a)anthracene	>	0.97713	=	0.78855	>	0.99724	>	0.98621	>	0.96305
chrysene	=	0.14883	>	0.99784	=	0.91853	=	0.79242	=	0.37657
benzo(b)flouranthene	=	0.47095	=	0.96549	=	0.99577	=	0.97058	=	0.90063
benzo(k)flouranthene	>	0.97240	>	0.99757	=	0.99606	=	0.97519	>	0.97891
benzo(e)pyrene	=	0.20424	=	0.97745	>	0.99870	=	0.98121	=	0.91525
benzo(a)pyrene	>	0.95573	>	0.99391	>	0.99824	=	0.97212	>	0.97184
indeno(123cd)pyrene	na		>	0.99650	>	0.99854	>	0.98835	>	0.97401
dibenzo(ah)anthracene	>	0.96428	>	0.98639	>	0.99061	>	0.95804	>	0.86619
benzo(ghi)perylene	=	0.55042	>	0.99693	>	0.99866	>	0.99543	>	0.97965

Table C.4.(3)

## Data from Gustafson and Dickhut (1997)

(supplementary information)

value to use for ND =	HAVEN	HAVEN	HAVEN	HAVEN	HAVEN	HAVEN	HAVEN
<b>0.3</b>	BEACH	BEACH	BEACH	BEACH	BEACH	BEACH	BEACH
pg/m <sup>3</sup> (avg value per article)	30-Jun-94	28-Jul-94	25-Aug-94	26-Sep-94	28-Oct-94		
	det- pg/m <sup>3</sup>	det- pg/m <sup>3</sup>					
	ect? gas phase	ect? gas phase					
fluorene	1 255.82	1 729.39	1 224.33	1 782.74	1 942.47		
phenanthrene	1 2748.83	1 4784.67	1 1291.99	1 1076.28	1 1936.58		
anthracene	1 69.31	1 83.91	1 21.54	nq	0 <b>0.30</b>		
fluoranthene	1 430.2	1 577.14	1 167.59	1 97.98	1 433.65		
pyrene	1 650.56	1 902.11	1 308.32	1 160.98	1 519.49		
benzo(a)anthracene	0 <b>0.30</b>	0 <b>0.30</b>	0 <b>0.30</b>	nq	1 13.2		
chrysene	1 27.9	1 33.76	1 13.27	1 7.87	1 110.02		
benzo(b)flouranthene	0 <b>0.30</b>	1 13.64	1 3.23	1 2.49	1 9.05		
benzo(k)flouranthene	0 <b>0.30</b>	0 <b>0.30</b>	0 <b>0.30</b>	0 <b>0.30</b>	1 4.62		
benzo(e)pyrene	0 <b>0.30</b>	1 9.97	1 7.37	1 1.41	1 5.37		
benzo(a)pyrene	0 <b>0.30</b>	1 6.36	1 1.38	nq	0 <b>0.30</b>		
indeno(123cd)pyrene	0 <b>0.30</b>						
dibenzo(ah)anthracene	0 <b>0.30</b>	0 <b>0.30</b>	1 0.6	0 <b>0.30</b>	0 <b>0.30</b>		
benzo(ghi)perylene	0 <b>0.30</b>	1 32.31	1 19.8	0 <b>0.30</b>	1 5.62		
///	///	///	///	///	///	///	///
	det- pg/m <sup>3</sup>						
	ect? particle phase						
fluorene	1 2.520	1 2.436	1 2.281	1 9.816	1 15.901		
phenanthrene	1 16.787	1 17.870	1 17.097	1 48.746	1 205.168		
anthracene	1 1.101	1 0.990	1 0.897	0 <b>0.300</b>	1 7.473		
fluoranthene	1 16.545	1 12.081	1 14.457	1 20.149	1 152.213		
pyrene	1 12.086	1 14.003	1 16.662	1 25.512	1 149.591		
benzo(a)anthracene	1 3.055	0 <b>0.300</b>	1 2.653	0 <b>0.300</b>	1 56.979		
chrysene	1 8.801	1 7.491	1 11.349	1 33.383	1 413.691		
benzo(b)flouranthene	1 6.748	1 7.901	1 10.434	1 63.298	1 322.224		
benzo(k)flouranthene	1 4.109	1 4.636	1 4.598	0 <b>0.300</b>	1 222.406		
benzo(e)pyrene	1 7.023	1 8.826	1 8.345	1 35.634	1 254.591		
benzo(a)pyrene	1 3.117	1 1.822	1 2.883	1 4.693	1 81.514		
indeno(123cd)pyrene	1 4.319	1 3.398	1 5.657	1 7.004	1 116.552		
dibenzo(ah)anthracene	1 0.973	1 0.726	1 1.739	1 2.057	1 16.395		
benzo(ghi)perylene	1 5.510	1 6.661	1 5.848	1 11.527	1 135.948		
///	///	///	///	///	///	///	///
	fraction in particle phase						
fluorene	= 0.00975	= 0.00333	= 0.01007	= 0.01239	= 0.01659		
phenanthrene	= 0.00607	= 0.00372	= 0.01306	= 0.04333	= 0.09579		
anthracene	= 0.01564	= 0.01166	= 0.03998	na	> 0.96140		
fluoranthene	= 0.03703	= 0.02050	= 0.07941	= 0.17057	= 0.25981		
pyrene	= 0.01824	= 0.01529	= 0.05127	= 0.13680	= 0.22358		
benzo(a)anthracene	> 0.91058	na	> 0.89841	na	= 0.81191		
chrysene	= 0.23980	= 0.18160	= 0.46099	= 0.80923	= 0.78992		
benzo(b)flouranthene	> 0.95743	= 0.36679	= 0.76361	= 0.96215	= 0.97268		
benzo(k)flouranthene	> 0.93196	> 0.93922	> 0.93875	na	= 0.97965		
benzo(e)pyrene	> 0.95903	= 0.46957	= 0.53102	= 0.96194	= 0.97934		
benzo(a)pyrene	> 0.91220	= 0.22268	= 0.67628	NQ	> 0.99633		
indeno(123cd)pyrene	> 0.93505	> 0.91888	> 0.94964	> 0.95893	> 0.99743		
dibenzo(ah)anthracene	> 0.76434	> 0.70760	= 0.74348	> 0.87272	> 0.98203		
benzo(ghi)perylene	> 0.94836	= 0.17092	= 0.22801	> 0.97463	= 0.96030		
=====	=====	=====	=====	=====	=====	=====	=====

Table C.4.(3)

## Data from Gustafson and Dickhut (1997)

(supplementary information)

value to use for ND =	HAVEN	HAVEN	HAVEN	HAVEN	HAVEN	HAVEN	HAVEN
<b>0.3</b>	BEACH	BEACH	BEACH	BEACH	BEACH	BEACH	BEACH
pg/m3 (avg value per article)	01-Dec-94	13-Jan-95	27-Jan-95	23-Feb-95	06-Apr-95		
	det- pg/m3						
	ect? gas phase						
fluorene	1 961.19	1 1277.53	1 1919.33	1 1813.15	1 1038.75		
phenanthrene	1 523.98	1 2329.37	1 2199.9	1 1843.46	1 901.1		
anthracene	0 <b>0.30</b>						
fluoranthene	1 114.18	1 359.29	1 323.17	1 507.26	1 190.4		
pyrene	1 62.88	1 417.78	1 169.11	1 198.26	1 100.65		
benzo(a)anthracene	1 6.56	1 3.3	0 <b>0.30</b>	0 <b>0.30</b>	0 <b>0.30</b>	0 <b>0.30</b>	
chrysene	1 28.86	1 34.48	1 7.15	1 16.89	1 16.44		
benzo(b)flouranthene	1 9.47	1 3.36	0 <b>0.30</b>	1 0.93	1 1.7		
benzo(k)flouranthene	1 7.91	1 2.81	0 <b>0.30</b>	0 <b>0.30</b>	1 0.62		
benzo(e)pyrene	1 6.18	1 2.58	0 <b>0.30</b>	1 0.58	1 1.02		
benzo(a)pyrene	0 <b>0.30</b>						
indeno(123cd)pyrene	0 <b>0.30</b>						
dibenzo(ah)anthracene	0 <b>0.30</b>						
benzo(ghi)perylene	0 <b>0.30</b>	1 1.84	0 <b>0.30</b>	0 <b>0.30</b>	1 0.8		
fluorene	1 3.750	nq	1 9.890	1 12.044	1 4.768		
phenanthrene	1 59.855	1 10.499	1 124.374	1 173.210	1 48.086		
anthracene	1 4.305	0 <b>0.300</b>	1 7.309	1 8.167	0 <b>0.300</b>		
fluoranthene	1 90.511	1 7.555	1 202.873	1 218.824	1 96.263		
pyrene	1 67.363	1 7.530	1 166.673	1 153.065	1 60.623		
benzo(a)anthracene	1 31.850	0 <b>0.300</b>	1 84.251	1 53.118	1 13.286		
chrysene	1 72.050	1 11.572	1 201.870	1 156.003	1 77.419		
benzo(b)flouranthene	1 116.755	1 8.993	1 306.389	1 190.353	1 102.188		
benzo(k)flouranthene	1 87.332	1 6.237	1 265.667	1 151.233	1 72.411		
benzo(e)pyrene	1 81.282	1 6.313	1 213.795	1 128.535	1 71.228		
benzo(a)pyrene	1 55.222	1 3.113	1 174.100	1 100.862	1 26.738		
indeno(123cd)pyrene	1 83.171	1 5.766	1 229.410	1 127.890	1 48.807		
dibenzo(ah)anthracene	1 11.719	1 0.838	1 28.642	1 16.986	1 3.975		
benzo(ghi)perylene	1 79.027	1 6.818	1 220.831	1 131.981	1 56.387		
fraction in			fraction in				
particle phase			particle phase				
fluorene	= 0.00389	<b>NQ</b>	= 0.00513	= 0.00660	= 0.00457		
phenanthrene	= 0.10252	= 0.00449	= 0.05351	= 0.08589	= 0.05066		
anthracene	> 0.93485	<b>na</b>	> 0.96057	> 0.96457	<b>na</b>		
fluoranthene	= 0.44218	= 0.02059	= 0.38566	= 0.30138	= 0.33581		
pyrene	= 0.51721	= 0.01770	= 0.49637	= 0.43568	= 0.37590		
benzo(a)anthracene	= 0.82921	< 0.08333	> 0.99645	> 0.99438	> 0.97792		
chrysene	= 0.71400	= 0.25128	= 0.96579	= 0.90231	= 0.82484		
benzo(b)flouranthene	= 0.92498	= 0.72800	> 0.99902	= 0.99514	= 0.98364		
benzo(k)flouranthene	= 0.91695	= 0.68940	> 0.99887	> 0.99802	= 0.99151		
benzo(e)pyrene	= 0.92934	= 0.70988	> 0.99860	= 0.99551	= 0.98588		
benzo(a)pyrene	> 0.99460	> 0.91210	> 0.99828	> 0.99703	> 0.98890		
indeno(123cd)pyrene	> 0.99641	> 0.95054	> 0.99869	> 0.99766	> 0.99389		
dibenzo(ah)anthracene	> 0.97504	> 0.73638	> 0.98963	> 0.98264	> 0.92982		
benzo(ghi)perylene	> 0.99622	= 0.78748	> 0.99864	> 0.99773	= 0.98601		

Table C.4.(3)

## Data from Gustafson and Dickhut (1997)

(supplementary information)

value to use for ND =	HAVEN	HAVEN	YORK	YORK	YORK
<b>0.3</b>	BEACH	BEACH	RIVER	RIVER	RIVER
pg/m <sup>3</sup> (avg value per article)	01-May-95	22-May-95	12-Aug-94	06-Oct-94	06-Dec-94
	det- pg/m <sup>3</sup>				
	ect? gas phase				
fluorene	1 487.27	1 390.6	1 4764.90	1 9638.81	1 15377.24
phenanthrene	1 516.14	1 1083.27	1 65243.00	1 21219.87	1 28183.18
anthracene	0 <b>0.30</b>	1 36.96	1 3234.85	1 1153.42	1 2424.90
fluoranthene	1 116.97	1 412.89	1 8056.13	1 3992.61	1 5338.88
pyrene	1 82.25	1 307.88	1 3067.21	1 1826.02	1 2631.84
benzo(a)anthracene	0 <b>0.30</b>	0 <b>0.30</b>	1 48.36	1 30.14	1 182.93
chrysene	1 8.91	1 19.96	1 157.35	1 75.03	1 364.72
benzo(b)flouranthene	1 1.45	1 1.4	1 67.52	1 15.15	1 63.36
benzo(k)flouranthene	1 0.8	0 <b>0.30</b>	0 <b>0.30</b>	0 <b>0.30</b>	1 71.35
benzo(e)pyrene	1 0.93	1 0.75	1 25.21	1 19.83	1 47.96
benzo(a)pyrene	0 <b>0.30</b>	0 <b>0.30</b>	1 8.68	1 11.30	1 14.57
indeno(123cd)pyrene	0 <b>0.30</b>	0 <b>0.30</b>	1 4.94	0 <b>0.30</b>	0 <b>0.30</b>
dibenzo(ah)anthracene	0 <b>0.30</b>	0 <b>0.30</b>	0 <b>0.30</b>	0 <b>0.30</b>	1 2.81
benzo(ghi)perylene	0 <b>0.30</b>	0 <b>0.30</b>	1 5.00	0 <b>0.30</b>	1 6.44
fluorene	nq	1 3.558	1 4.001	1 33.787	1 13.905
phenanthrene	nq	1 31.549	1 29.484	1 282.348	1 108.587
anthracene	0 <b>0.300</b>	1 2.604	1 3.115	1 19.191	1 13.905
fluoranthene	1 2.335	1 49.257	1 32.765	1 203.452	1 98.235
pyrene	1 1.512	1 36.161	1 20.058	1 157.649	1 94.720
benzo(a)anthracene	1 1.627	1 12.328	1 6.518	1 75.405	1 62.300
chrysene	1 2.211	1 37.856	1 18.034	1 166.363	1 136.365
benzo(b)flouranthene	1 1.962	1 38.805	1 17.752	1 292.194	1 386.033
benzo(k)flouranthene	1 1.390	1 27.149	1 12.714	1 221.273	1 332.469
benzo(e)pyrene	1 1.266	1 26.320	1 7.795	1 234.671	1 358.517
benzo(a)pyrene	1 0.833	1 20.766	1 7.353	1 125.562	1 138.628
indeno(123cd)pyrene	0 <b>0.300</b>	1 21.473	1 20.425	1 196.521	1 584.253
dibenzo(ah)anthracene	0 <b>0.300</b>	1 3.197	1 3.407	1 25.043	1 36.655
benzo(ghi)perylene	0 <b>0.300</b>	1 24.121	1 29.530	1 261.975	1 746.305
fluorene	<b>NQ</b>	= 0.00903	= 0.00084	= 0.00349	= 0.00090
phenanthrene	<b>NQ</b>	= 0.02830	= 0.00045	= 0.01313	= 0.00384
anthracene	<b>na</b>	= 0.06582	= 0.00096	= 0.01637	= 0.00570
fluoranthene	= 0.01957	= 0.10658	= 0.00405	= 0.04849	= 0.01807
pyrene	= 0.01805	= 0.10511	= 0.00650	= 0.07947	= 0.03474
benzo(a)anthracene	> 0.84432	> 0.97624	= 0.11877	= 0.71443	= 0.25405
chrysene	= 0.19881	= 0.65477	= 0.10283	= 0.68918	= 0.27214
benzo(b)flouranthene	= 0.57503	= 0.96518	= 0.20818	= 0.95071	= 0.85901
benzo(k)flouranthene	= 0.63470	> 0.98907	> 0.97695	> 0.99865	= 0.82331
benzo(e)pyrene	= 0.57650	= 0.97229	= 0.23618	= 0.92208	= 0.88201
benzo(a)pyrene	> 0.73522	> 0.98576	= 0.45862	= 0.91744	= 0.90489
indeno(123cd)pyrene	<b>na</b>	> 0.98622	= 0.80524	> 0.99848	> 0.99949
dibenzo(ah)anthracene	<b>na</b>	> 0.91421	> 0.91907	> 0.98816	= 0.92880
benzo(ghi)perylene	<b>na</b>	> 0.98772	= 0.85520	> 0.99886	= 0.99144

Table C.4.(3)

## Data from Gustafson and Dickhut (1997)

(supplementary information)

value to use for ND =	YORK	YORK	YORK	YORK	YORK	YORK	YORK
<b>0.3</b>	RIVER	RIVER	RIVER	RIVER	RIVER	RIVER	RIVER
pg/m <sup>3</sup> (avg value per article)	07-Dec-94	09-Dec-94	10-Feb-95	12-Apr-95	24-May-95		
	det- pg/m <sup>3</sup>	det- pg/m <sup>3</sup>					
	ect? gas phase	ect? gas phase					
fluorene	1 9000.11	1 3885.72	1 5714.64	1 6557.20	1 16420.99		
phenanthrene	1 21384.75	1 8782.73	1 5925.09	1 16133.94	1 31113.35		
anthracene	1 932.55	1 317.48	1 151.80	1 267.26	1 595.91		
fluoranthene	1 5795.52	1 1438.16	1 1488.32	1 2189.64	1 5019.09		
pyrene	1 2350.18	1 978.73	1 506.78	1 785.96	1 1467.32		
benzo(a)anthracene	1 38.96	1 12.89	0 <b>0.30</b>	1 8.00	1 18.34		
chrysene	1 177.40	1 71.57	1 47.42	1 64.50	1 97.85		
benzo(b)flouranthene	1 12.07	1 4.42	1 3.63	1 7.76	1 6.97		
benzo(k)flouranthene	0 <b>0.30</b>	0 <b>0.30</b>	0 <b>0.30</b>	1 4.86	1 3.29		
benzo(e)pyrene	1 7.89	1 2.74	1 1.41	1 5.06	1 4.34		
benzo(a)pyrene	1 3.04	0 <b>0.30</b>	0 <b>0.30</b>	1 2.88	0 <b>0.30</b>		
indeno(123cd)pyrene	0 <b>0.30</b>	0 <b>0.30</b>	0 <b>0.30</b>	1 4.85	0 <b>0.30</b>		
dibenzo(ah)anthracene	0 <b>0.30</b>	0 <b>0.30</b>	0 <b>0.30</b>	1 0.95	0 <b>0.30</b>		
benzo(ghi)perylene	1 12.11	1 1.39	1 1.10	1 5.27	0 <b>0.30</b>		
///	///	///	///	///	///	///	///
	det- pg/m <sup>3</sup>						
	ect? particle phase						
fluorene	1 4.910	1 7.030	1 4.495	nq		1 15.278	
phenanthrene	1 51.958	1 86.516	1 65.786	1 19.892	1 82.177		
anthracene	1 3.334	1 6.543	1 4.162	1 1.063	1 6.277		
fluoranthene	1 55.919	1 135.613	1 119.632	1 24.635	1 105.852		
pyrene	1 43.647	1 126.910	1 86.654	1 15.626	1 109.704		
benzo(a)anthracene	1 20.143	1 56.771	1 26.381	1 5.199	0 <b>0.30</b>		
chrysene	1 53.127	1 156.929	1 87.392	1 14.094	1 79.359		
benzo(b)flouranthene	1 80.040	1 165.008	1 116.123	1 13.453	1 51.104		
benzo(k)flouranthene	1 66.081	1 131.444	1 85.991	1 9.678	1 29.249		
benzo(e)pyrene	1 64.860	1 133.200	1 77.324	1 9.171	1 60.762		
benzo(a)pyrene	1 37.374	1 89.722	1 41.656	1 6.098	1 22.264		
indeno(123cd)pyrene	1 75.998	1 139.859	1 88.177	1 7.172	1 24.444		
dibenzo(ah)anthracene	1 6.635	1 14.765	1 9.574	1 1.682	0 <b>0.30</b>		
benzo(ghi)perylene	1 90.836	1 186.523	1 88.744	1 8.638	1 48.817		
///	///	///	///	///	///	///	///
	fraction in particle phase						
fluorene	= 0.00055	= 0.00181	= 0.00079	<b>NQ</b>		= 0.00093	
phenanthrene	= 0.00242	= 0.00975	= 0.01098	= 0.00123	= 0.00263		
anthracene	= 0.00356	= 0.02019	= 0.02669	= 0.00396	= 0.01042		
fluoranthene	= 0.00956	= 0.08617	= 0.07440	= 0.01113	= 0.02065		
pyrene	= 0.01823	= 0.11478	= 0.14602	= 0.01949	= 0.06956		
benzo(a)anthracene	= 0.34081	= 0.81496	> 0.98876	= 0.39389	< 0.01609		
chrysene	= 0.23046	= 0.68678	= 0.64825	= 0.17933	= 0.44783		
benzo(b)flouranthene	= 0.86896	= 0.97391	= 0.96969	= 0.63419	= 0.87998		
benzo(k)flouranthene	> 0.99548	> 0.99772	> 0.99652	= 0.66570	= 0.89889		
benzo(e)pyrene	= 0.89155	= 0.97984	= 0.98209	= 0.64444	= 0.93334		
benzo(a)pyrene	= 0.92478	> 0.99667	> 0.99285	= 0.67922	> 0.98670		
indeno(123cd)pyrene	> 0.99607	> 0.99786	> 0.99661	= 0.59657	> 0.98788		
dibenzo(ah)anthracene	> 0.95674	> 0.98009	> 0.96962	= 0.63906	<b>na</b>		
benzo(ghi)perylene	= 0.88237	= 0.99260	= 0.98776	= 0.62108	> 0.99389		

Table C.4.(3)

## Data from Gustafson and Dickhut (1997)

(supplementary information)

value to use for ND =	HAVEN	HAVEN	HAVEN	HAVEN	HAVEN	HAVEN	HAVEN			
<b>0.3</b>	BEACH	BEACH	BEACH	BEACH	BEACH	BEACH	BEACH			
pg/m <sup>3</sup> (avg value per article)	10-May-94	22-May-94	26-Jun-94	28-Jun-94	29-Jun-94					
	det- pg/m <sup>3</sup>	det- pg/m <sup>3</sup>								
	ect? gas phase	ect? gas phase								
fluorene	1	731.33	1	671.62	1	439.96	1	725.87	1	376.65
phenanthrene	1	1914.11	1	1718.83	1	3711.71	1	4227.41	1	3688.97
anthracene	0	<b>0.30</b>	0	<b>0.30</b>	0	<b>0.30</b>	0	<b>0.30</b>	1	54.50
fluoranthene	1	353.22	1	305.98	1	416.55	1	630.83	1	492.20
pyrene	1	451.54	1	277.54	1	512.98	1	984.84	1	556.21
benzo(a)anthracene	0	<b>0.30</b>	0	<b>0.30</b>	0	<b>0.30</b>	0	<b>0.30</b>	0	<b>0.30</b>
chrysene	1	25.69	1	12.80	1	42.71	1	41.60	1	39.90
benzo(b)flouranthene	1	4.36	1	1.34	1	3.32	0	<b>0.30</b>	1	5.30
benzo(k)flouranthene	0	<b>0.30</b>	1	0.62	0	<b>0.30</b>	0	<b>0.30</b>	1	1.47
benzo(e)pyrene	1	1.89	1	1.01	1	7.76	0	<b>0.30</b>	1	4.56
benzo(a)pyrene	0	<b>0.30</b>	0	<b>0.30</b>	1	1.16	0	<b>0.30</b>	1	1.53
indeno(123cd)pyrene	0	<b>0.30</b>	0	<b>0.30</b>	0	<b>0.30</b>	0	<b>0.30</b>	0	<b>0.30</b>
dibenzo(ah)anthracene	0	<b>0.30</b>	0	<b>0.30</b>	0	<b>0.30</b>	0	<b>0.30</b>	1	3.40
benzo(ghi)perylene	0	<b>0.30</b>	0	<b>0.30</b>	1	3.02	0	<b>0.30</b>	1	5.58
///	///	///	///	///	///	///	///	///	///	///
	det- pg/m <sup>3</sup>	det- pg/m <sup>3</sup>								
	ect?particle phase	ect?particle phase								
fluorene	1	4.757	1	3.302	1	2.340	1	3.339	1	1.548
phenanthrene	1	42.833	1	32.010	1	14.953	1	28.781	1	13.196
anthracene	1	4.703	1	2.802	1	1.237	1	2.821	1	1.173
fluoranthene	1	47.474	1	43.728	1	11.406	1	25.359	1	13.055
pyrene	1	40.760	1	35.818	1	9.524	1	22.778	1	9.644
benzo(a)anthracene	1	17.539	1	13.286	1	3.207	1	7.948	1	3.939
chrysene	1	46.751	1	36.720	1	8.227	1	16.748	1	9.475
benzo(b)flouranthene	1	83.156	1	35.105	1	7.937	1	14.150	1	9.124
benzo(k)flouranthene	1	69.140	1	24.431	1	5.506	1	10.290	1	9.324
benzo(e)pyrene	1	77.831	1	28.713	1	7.703	1	13.321	1	8.852
benzo(a)pyrene	1	39.360	1	15.296	1	3.595	1	8.134	1	4.451
indeno(123cd)pyrene	1	74.710	1	22.485	1	5.415	1	9.151	1	7.155
dibenzo(ah)anthracene	1	10.876	1	3.980	1	2.228	1	1.881	1	1.416
benzo(ghi)perylene	1	81.975	1	28.505	1	6.813	1	11.433	1	8.606
///	///	///	///	///	///	///	///	///	///	///
	fraction in particle phase									
fluorene	=	0.00646	=	0.00489	=	0.00529	=	0.00458	=	0.00409
phenanthrene	=	0.02189	=	0.01828	=	0.00401	=	0.00676	=	0.00356
anthracene	>	0.94004	>	0.90329	>	0.80481	>	0.90388	=	0.02107
fluoranthene	=	0.11848	=	0.12504	=	0.02665	=	0.03865	=	0.02584
pyrene	=	0.08280	=	0.11430	=	0.01823	=	0.02261	=	0.01704
benzo(a)anthracene	>	0.98318	>	0.97792	>	0.91446	>	0.96363	>	0.92923
chrysene	=	0.64537	=	0.74152	=	0.16151	=	0.28704	=	0.19190
benzo(b)flouranthene	=	0.95018	=	0.96323	=	0.70507	>	0.97924	=	0.63256
benzo(k)flouranthene	>	0.99568	=	0.97525	>	0.94833	>	0.97167	=	0.86381
benzo(e)pyrene	=	0.97629	=	0.96602	=	0.49816	>	0.97798	=	0.66001
benzo(a)pyrene	>	0.99244	>	0.98076	=	0.75605	>	0.96443	=	0.74419
indeno(123cd)pyrene	>	0.99600	>	0.98683	>	0.94751	>	0.96826	>	0.95976
dibenzo(ah)anthracene	>	0.97316	>	0.92991	>	0.88133	>	0.86245	=	0.29402
benzo(ghi)perylene	>	0.99635	>	0.98959	=	0.69287	>	0.97443	=	0.60665
=====	=====	=====	=====	=====	=====	=====	=====	=====	=====	=====

Table C.4.(3)

## Data from Gustafson and Dickhut (1997)

(supplementary information)

value to use for ND =	HAVEN	HAVEN	ELIZABETH	ELIZABETH	ELIZABETH
0.3	BEACH	BEACH	RIVER	RIVER	RIVER
pg/m <sup>3</sup> (avg value per article)	05-Nov-94	08-Nov-94	15-Jul-94	08-Sep-94	12-Nov-94
	det- pg/m <sup>3</sup>				
	ect? gas phase				
fluorene	1 799.66	1 1007.10	nq	1 5056.24	1 8333.31
phenanthrene	1 2300.57	1 2518.09	nq	1 17823.32	1 12894.94
anthracene	1 123.35	0 <b>0.30</b>	nq	1 869.63	1 281.96
fluoranthene	1 432.38	1 363.83	nq	1 4576.92	1 1794.26
pyrene	1 419.17	1 411.92	nq	1 2524.15	1 1209.90
benzo(a)anthracene	1 9.69	1 9.07	1 284.27	1 29.25	1 10.96
chrysene	1 56.78	1 74.57	1 1812.49	1 141.08	1 68.78
benzo(b)flouranthene	1 11.95	1 13.01	1 10.79	1 19.43	1 5.90
benzo(k)flouranthene	0 <b>0.30</b>	0 <b>0.30</b>	0 <b>0.30</b>	1 17.81	1 2.90
benzo(e)pyrene	1 106.62	1 13.53	0 <b>0.30</b>	1 15.73	1 5.63
benzo(a)pyrene	1 4.66	1 3.64	1 66.95	1 9.05	0 <b>0.30</b>
indeno(123cd)pyrene	0 <b>0.30</b>	0 <b>0.30</b>	1 6.84	0 <b>0.30</b>	0 <b>0.30</b>
dibenzo(ah)anthracene	0 <b>0.30</b>				
benzo(ghi)perylene	1 15.00	1 14.17	1 10.77	0 <b>0.30</b>	1 7.57
///	///	///	///	///	///
	det- pg/m <sup>3</sup>				
	ect?particle phase				
fluorene	1 3.446	1 4.684	1 7.020	1 11.013	1 10.203
phenanthrene	1 24.101	1 42.327	1 43.053	1 96.969	1 91.788
anthracene	1 1.559	1 2.432	1 3.340	1 14.045	1 5.202
fluoranthene	1 16.101	1 51.709	1 20.530	1 96.673	1 125.574
pyrene	1 13.809	1 76.827	1 16.898	1 66.061	1 96.971
benzo(a)anthracene	1 6.672	1 52.259	1 6.263	1 25.930	1 29.994
chrysene	1 19.495	1 122.188	1 21.719	1 74.070	1 82.156
benzo(b)flouranthene	1 30.932	1 64.173	1 17.122	1 76.709	1 87.384
benzo(k)flouranthene	1 23.166	1 36.751	1 8.885	1 59.517	1 71.376
benzo(e)pyrene	1 22.596	1 61.696	1 13.190	1 55.687	1 65.189
benzo(a)pyrene	1 8.216	1 23.995	1 6.539	1 33.368	1 48.235
indeno(123cd)pyrene	1 18.009	1 43.548	1 10.645	1 48.811	1 68.601
dibenzo(ah)anthracene	1 3.060	1 5.406	0 <b>0.30</b>	1 7.321	1 10.669
benzo(ghi)perylene	1 17.821	1 55.657	1 18.206	1 54.589	1 89.452
///	///	///	///	///	///
	fraction in particle phase				
fluorene	= 0.00429	= 0.00463	NQ	= 0.00217	= 0.00122
phenanthrene	= 0.01037	= 0.01653	NQ	= 0.00541	= 0.00707
anthracene	= 0.01248	> 0.89019	NQ	= 0.01589	= 0.01812
fluoranthene	= 0.03590	= 0.12444	NQ	= 0.02068	= 0.06541
pyrene	= 0.03189	= 0.15719	NQ	= 0.02550	= 0.07420
benzo(a)anthracene	= 0.40777	= 0.85211	= 0.02156	= 0.46992	= 0.73238
chrysene	= 0.25559	= 0.62101	= 0.01184	= 0.34427	= 0.54431
benzo(b)flouranthene	= 0.72133	= 0.83144	= 0.61343	= 0.79790	= 0.93675
benzo(k)flouranthene	> 0.98722	> 0.99190	> 0.96734	= 0.76968	= 0.96096
benzo(e)pyrene	= 0.17487	= 0.82014	> 0.97776	= 0.77974	= 0.92050
benzo(a)pyrene	= 0.63809	= 0.86828	= 0.08898	= 0.78665	> 0.99382
indeno(123cd)pyrene	> 0.98361	> 0.99316	= 0.60881	> 0.99389	> 0.99565
dibenzo(ah)anthracene	> 0.91071	> 0.94742	na	> 0.96064	> 0.97265
benzo(ghi)perylene	= 0.54298	= 0.79707	= 0.62831	> 0.99453	= 0.92198
=====	=====	=====	=====	=====	=====

Table C.4.(3)

## Data from Gustafson and Dickhut (1997)

(supplementary information)

value to use for ND =	ELIZABETH	ELIZABETH	ELIZABETH	HAMPTON	HAMPTON	
0.3	RIVER	RIVER	RIVER			
pg/m <sup>3</sup> (avg value per article)	09-Jan-95	11-Mar-95	04-May-95	15-Jul-94	09-Sep-94	
	det- pg/m <sup>3</sup>					
	ect? gas phase					
fluorene	1 5741.74	1 2788.34	1 11204.46	1 29218.03	1 24670.86	
phenanthrene	1 11515.13	1 6013.35	1 25225.86	1 124573.46	1 80242.93	
anthracene	1 750.63	1 124.01	1 1042.99	1 6939.02	1 2526.69	
fluoranthene	1 1607.14	1 677.71	1 3901.73	1 12854.70	1 4080.84	
pyrene	1 1629.53	1 500.74	1 2018.29	1 5559.62	1 1678.95	
benzo(a)anthracene	1 12.94	0 <b>0.30</b>	1 35.48	1 24.99	1 10.37	
chrysene	1 42.42	1 15.07	1 91.78	1 144.95	1 49.05	
benzo(b)flouranthene	1 6.92	1 1.77	1 10.47	1 16.31	1 16.60	
benzo(k)flouranthene	1 4.53	1 1.74	1 6.60	0 <b>0.30</b>	0 <b>0.30</b>	
benzo(e)pyrene	1 5.76	0 <b>0.30</b>	1 5.67	1 15.56	1 6.76	
benzo(a)pyrene	1 3.71	0 <b>0.30</b>	1 4.17	1 1.55	0 <b>0.30</b>	
indeno(123cd)pyrene	1 4.72	0 <b>0.30</b>	1 6.62	0 <b>0.30</b>	0 <b>0.30</b>	
dibenzo(ah)anthracene	0 <b>0.30</b>	0 <b>0.30</b>	1 9.77	0 <b>0.30</b>	0 <b>0.30</b>	
benzo(ghi)perylene	1 8.93	0 <b>0.30</b>	1 10.07	0 <b>0.30</b>	0 <b>0.30</b>	
	=====	=====	=====	=====	=====	
	det- pg/m <sup>3</sup>					
	ect? particle phase					
fluorene	1 20.671	1 8.870	1 14.098	1 11.708	1 21.773	
phenanthrene	1 302.056	1 169.838	1 130.250	1 70.994	1 155.231	
anthracene	1 36.721	1 8.170	1 8.561	1 5.270	1 15.271	
fluoranthene	1 533.524	1 205.687	1 229.606	1 57.130	1 89.400	
pyrene	1 631.710	1 142.532	1 184.695	1 34.809	1 87.818	
benzo(a)anthracene	1 200.210	1 52.584	1 59.183	1 10.268	1 13.121	
chrysene	1 864.645	1 136.250	1 350.255	1 31.083	1 43.043	
benzo(b)flouranthene	1 433.885	1 155.686	1 150.210	1 23.428	1 53.833	
benzo(k)flouranthene	1 332.971	1 117.906	1 91.493	1 16.209	1 41.084	
benzo(e)pyrene	1 387.036	1 107.813	1 122.232	1 16.592	1 38.778	
benzo(a)pyrene	1 271.294	1 81.861	1 60.028	1 9.910	1 19.241	
indeno(123cd)pyrene	1 365.048	1 116.611	1 88.778	1 10.125	1 20.923	
dibenzo(ah)anthracene	1 43.623	1 13.676	1 29.596	0 <b>0.30</b>	0 <b>0.30</b>	
benzo(ghi)perylene	1 513.626	1 140.102	1 143.076	1 16.677	1 20.750	
	=====	=====	=====	=====	=====	
	fraction in particle phase					
fluorene	= 0.00359	= 0.00317	= 0.00126	= 0.00040	= 0.00088	
phenanthrene	= 0.02556	= 0.02747	= 0.00514	= 0.00057	= 0.00193	
anthracene	= 0.04664	= 0.06181	= 0.00814	= 0.00076	= 0.00601	
fluoranthene	= 0.24923	= 0.23284	= 0.05558	= 0.00442	= 0.02144	
pyrene	= 0.27936	= 0.22157	= 0.08384	= 0.00622	= 0.04971	
benzo(a)anthracene	= 0.93929	> 0.99433	= 0.62520	= 0.29122	= 0.55855	
chrysene	= 0.95323	= 0.90041	= 0.79237	= 0.17657	= 0.46739	
benzo(b)flouranthene	= 0.98430	= 0.98876	= 0.93484	= 0.58956	= 0.76432	
benzo(k)flouranthene	= 0.98658	= 0.98546	= 0.93272	> 0.98183	> 0.99275	
benzo(e)pyrene	= 0.98534	> 0.99723	= 0.95567	= 0.51605	= 0.85155	
benzo(a)pyrene	= 0.98651	> 0.99635	= 0.93504	= 0.86475	> 0.98465	
indeno(123cd)pyrene	= 0.98724	> 0.99743	= 0.93061	> 0.97122	> 0.98586	
dibenzo(ah)anthracene	> 0.99317	> 0.97853	= 0.75182	na	na	
benzo(ghi)perylene	= 0.98291	> 0.99786	= 0.93425	> 0.98233	> 0.98575	
	=====	=====	=====	=====	=====	

Table C.4.(3)

## Data from Gustafson and Dickhut (1997)

(supplementary information)

value to use for ND =	HAMPTON	HAMPTON	HAMPTON	HAMPTON	HAMPTON
<b>0.3</b>					
pg/m <sup>3</sup> (avg value per article)	12-Nov-94	09-Jan-95	11-Mar-95	04-May-95	
	det- pg/m <sup>3</sup>	det- pg/m <sup>3</sup>	det- pg/m <sup>3</sup>	det- pg/m <sup>3</sup>	
	ect? gas phase	ect? gas phase	ect? gas phase	ect? gas phase	
fluorene	1 1738.09	1 2417.97	1 4256.63	1 40581.78	
phenanthrene	1 2456.33	1 3598.42	1 10770.95	1 47281.54	
anthracene	0 <b>0.30</b>	1 197.56	0 <b>0.30</b>	1 1289.49	
fluoranthene	1 800.69	1 834.53	1 2301.69	1 8750.36	
pyrene	1 1131.33	1 567.93	1 952.30	1 2078.87	
benzo(a)anthracene	0 <b>0.30</b>	1 7.48	0 <b>0.30</b>	1 17.37	
chrysene	1 49.90	1 41.53	1 198.41	1 110.93	
benzo(b)flouranthene	1 2.50	1 2.33	1 14.39	1 14.90	
benzo(k)flouranthene	1 1.58	0 <b>0.30</b>	0 <b>0.30</b>	1 7.77	
benzo(e)pyrene	1 1.65	1 1.45	1 24.06	1 10.49	
benzo(a)pyrene	0 <b>0.30</b>	0 <b>0.30</b>	0 <b>0.30</b>	1 4.69	
indeno(123cd)pyrene	0 <b>0.30</b>	0 <b>0.30</b>	0 <b>0.30</b>	1 8.55	
dibenzo(ah)anthracene	0 <b>0.30</b>	0 <b>0.30</b>	0 <b>0.30</b>	0 <b>0.30</b>	
benzo(ghi)perylene	1 1.23	1 0.72	1 4.96	1 9.16	
///	///	///	///	///	///
	det- pg/m <sup>3</sup>	det- pg/m <sup>3</sup>	det- pg/m <sup>3</sup>	det- pg/m <sup>3</sup>	
	ect?particle phase	ect?particle phase	ect?particle phase	ect?particle phase	
fluorene	1 11.029	1 15.120	1 7.845	nq	
phenanthrene	1 81.170	1 167.214	1 111.240	1 16.709	
anthracene	1 3.569	1 11.042	1 9.082	1 0.826	
fluoranthene	1 138.903	1 214.940	1 156.416	1 12.088	
pyrene	1 135.126	1 146.144	1 105.690	1 10.363	
benzo(a)anthracene	1 21.559	1 178.023	1 47.569	0 <b>0.30</b>	
chrysene	1 79.058	1 192.490	1 121.683	1 11.097	
benzo(b)flouranthene	1 72.988	1 259.754	1 169.004	1 10.918	
benzo(k)flouranthene	1 44.208	1 208.361	1 119.757	1 7.865	
benzo(e)pyrene	1 52.897	1 171.040	1 106.809	1 7.827	
benzo(a)pyrene	1 32.684	1 131.059	1 77.120	1 4.953	
indeno(123cd)pyrene	1 34.230	1 193.042	1 101.563	1 7.393	
dibenzo(ah)anthracene	1 6.285	1 29.495	1 14.160	1 1.985	
benzo(ghi)perylene	1 46.531	1 183.864	1 113.417	1 10.486	
///	///	///	///	///	///
	fraction in particle phase				
fluorene	= 0.00631	= 0.00621	= 0.00184	<b>NQ</b>	
phenanthrene	= 0.03199	= 0.04441	= 0.01022	= 0.00035	
anthracene	> 0.92246	= 0.05293	> 0.96802	= 0.00064	
fluoranthene	= 0.14783	= 0.20481	= 0.06363	= 0.00138	
pyrene	= 0.10670	= 0.20466	= 0.09990	= 0.00496	
benzo(a)anthracene	> 0.98628	= 0.95968	> 0.99373	< 0.01698	
chrysene	= 0.61305	= 0.82254	= 0.38015	= 0.09094	
benzo(b)flouranthene	= 0.96688	= 0.99111	= 0.92154	= 0.42288	
benzo(k)flouranthene	= 0.96549	> 0.99856	> 0.99750	= 0.50304	
benzo(e)pyrene	= 0.96975	= 0.99159	= 0.81615	= 0.42731	
benzo(a)pyrene	> 0.99090	> 0.99772	> 0.99613	= 0.51364	
indeno(123cd)pyrene	> 0.99131	> 0.99845	> 0.99705	= 0.46371	
dibenzo(ah)anthracene	> 0.95444	> 0.98993	> 0.97925	> 0.86871	
benzo(ghi)perylene	= 0.97425	= 0.99610	= 0.95810	= 0.53375	
=====	=====	=====	=====	=====	

**Appendix D.**

**Atmospheric Fate Mechanisms**  
**and**  
**Atmospheric Lifetimes**

## Appendix D.1. Characteristic Time for Gas-Phase Washout by Wet Deposition from the Atmosphere

As discussed in Appendix C, compounds can exist in the vapor phase and/or the particle phase in the atmosphere. This analysis has used a simple form of vapor/particle partitioning theory to make qualitative estimates of this phenomenon. The extent to which a chemical exists in either phase at any given location in the atmosphere depends (at least) on the particular physical-chemical properties of the substance as well as the ambient temperature and the nature of the atmospheric aerosol.

One depletion mechanism for atmospheric pollutants is the removal of gas-phase pollutants by rainfall. For pollutants that have very limited water solubility, this mechanism will not be very significant.

A simplified approach was taken to make a qualitative estimate of the time scale for gas-phase washout of pollutants by wet deposition. This approach is described as follows.

The rate of deposition,  $W$  (g/m<sup>2</sup>-day), of a given compound is given by the product of the rainfall rate,  $J$  (m<sup>3</sup>/m<sup>2</sup>-day [=] m/day), the molar concentration of the pollutant in the rain  $C_{aq}$  (mol/m<sup>3</sup>), and the molecular weight of the substance  $m_w$  (g/mol):

$$(1) \quad W = J C_{aq} m_w$$

The total amount of a given compound in the atmosphere (per square meter of earth surface),  $M$  (g/m<sup>2</sup>), is given by product of the assumed height of the chemical layer in the atmosphere,  $L$  (m), and the concentration of pollutant in the atmosphere,  $C_g$  (atm):

$$(2) \quad M = L C_g (m_w / R T)$$

where the term in parentheses ( $m_w / RT$  = molecular weight / gas constant \* temperature) has been included for dimensional consistency.

A characteristic time for removal of a given pollutant by deposition can be defined as the mass of pollutant in the atmosphere divided by the rate of removal. In the case of wet deposition of gas-phase pollutants, this characteristic time —  $\tau_{w,g}$  — can be defined in terms of the above variables as:

$$(3) \quad \tau_{w,g} = M / W = L C_g (m_w / RT) / J C_{aq} m_w$$

Canceling  $m_w$  and rearranging, one obtains:

$$(4) \quad \tau_{w,g} = (L / J R T) (C_g / C_{aq})$$

Assuming equilibrium between the gas phase and aqueous phase and assuming that the atmospheric layer is well mixed, the gas- and aqueous-phase concentrations can be related using Henry's Law:

$$(5) \quad C_g(\text{atm}) = C_{aq} (\text{mol}/\text{m}^3) H (\text{atm}\cdot\text{m}^3/\text{mol})$$

where  $C_g$  is the gas phase concentration,  $C_{aq}$  is the aqueous phase concentration, and  $H$  is the Henry's Law Constant for the particular substance at the temperature of interest.

Substituting equation (5) into (4), one obtains the following expression for the characteristic time for removal of a given pollutant from the atmosphere by wet deposition of gas phase material:

$$(6) \quad \tau_{w,g} = H L / J R T$$

An example of a consistent set of units for using this equation, giving the characteristic time in days, is the following:

H	[=] atm-m <sup>3</sup> /mol
L	[=] m
J	[=] m/day
R	[=] 8.20575x10 <sup>-5</sup> m <sup>3</sup> atm (deg K) <sup>-1</sup> mol <sup>-1</sup>
T	[=] deg K

Calculations with equation (6) are shown in the figure below. For this figure, a temperature of 290 K was used, a rainfall rate of 30 inches per year (0.0021 m/day) was assumed, and the chemical layer height, L, ranged from 500 m to 10,000 m. It can be seen that compounds with Henry's Law Constants  $\leq 1 \times 10^{-8}$  atm-m<sup>3</sup>/mol can be fairly effectively removed from the atmosphere (e.g., with characteristic times of less than 1 day) to the extent that they exist in the gas phase. Compounds with Henry's Law Constants  $\geq 1 \times 10^{-5}$  atm-m<sup>3</sup>/mol will not be removed efficiently from the atmosphere by wet deposition of gas phase material. For compounds with Henry's Law Constants between  $1 \times 10^{-8}$  and  $1 \times 10^{-5}$ , wet deposition of gas phase material — to the extent that the compound exists in the gas phase at all -- may or may not be important.

An approximate way to combine the effects of vapor/particle partitioning into this estimation is to simply divide the estimated characteristic time by the typical fraction that exists in the vapor phase (estimated by the vapor/particle partitioning theory). That is, for example, if 100% of the compound exists in the vapor phase, then the V/P-adjusted characteristic time for gas-phase wet removal is  $\tau_{w,g} / 100\% = \tau_{w,g}^{(V/P)}$ ; if 1% of the compound exists in the vapor phase, then the V/P-adjusted characteristic time for gas-phase wet removal is  $\tau_{w,g} / 1\% = 100 \tau_{w,g}^{(V/P)}$ . This V/P-adjusted characteristic time will be denoted by  $\tau_{w,g}^{(V/P)}$ .

It is important to note that  $\tau_{w,g}^{(V/P)}$  is *not* an estimate of the atmospheric lifetime of a given compound relative to precipitation. It is simply a qualitative measure of the significance of this deposition pathway.

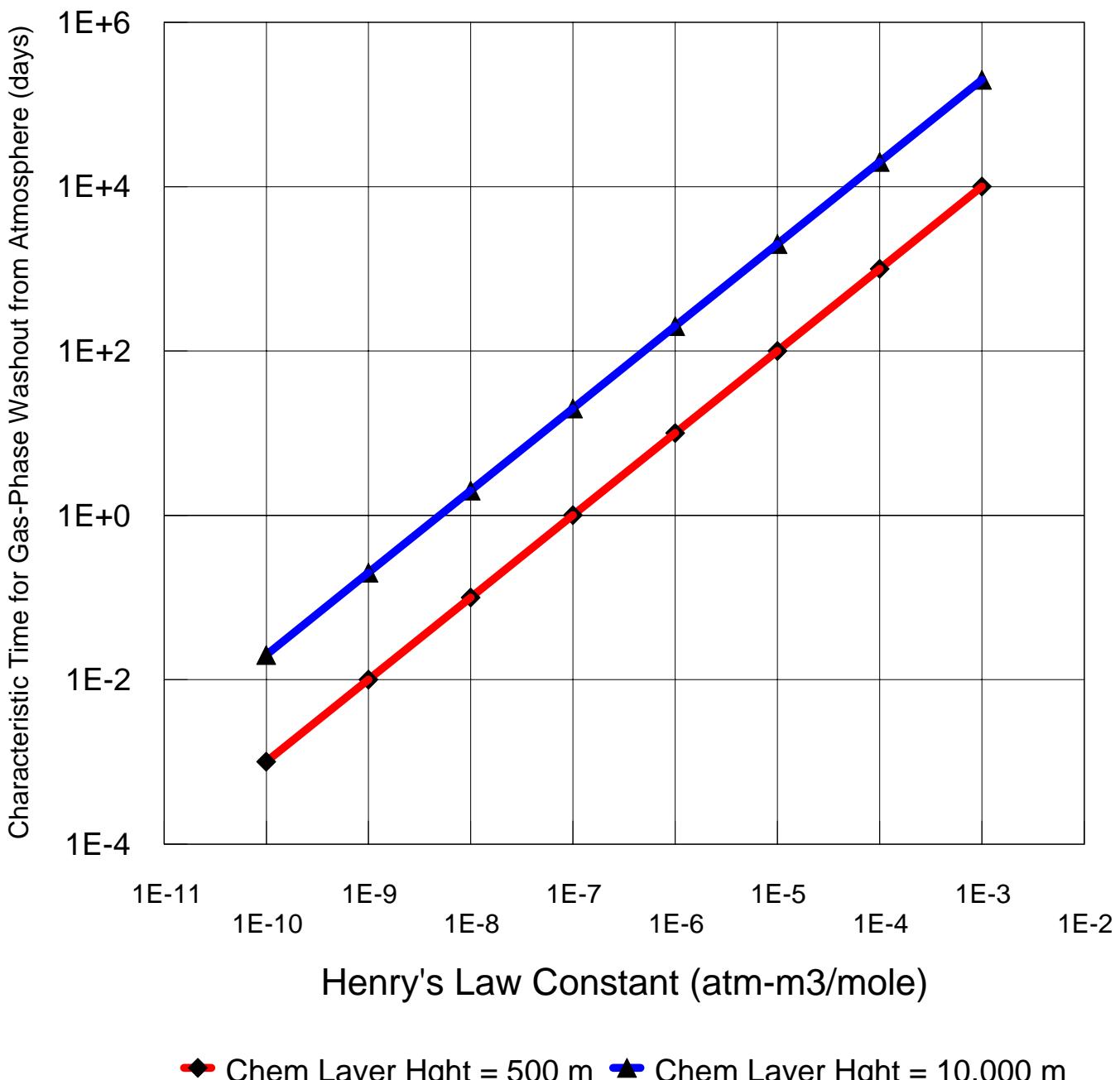
Estimates of  $\tau_{w,g}^{(V/P)}$  were made as many of the compounds considered in this analysis for which Henry's Law Constants and basic V/P partitioning estimates could be obtained. These estimates are presented in the table below.

For most of the compounds considered in this analysis,  $\tau_{w,g}^{(V/P)}$  is very large — on the order of 100-10,000 days. For one of the compounds -- 4,4'-methylene bis(2-chloroaniline, "MBOCA") —  $\tau_{w,g}^{(V/P)} \approx 4.1 \times 10^{-3}$  days  $\approx$  6 minutes, suggesting that this compound will be very effectively removed from the atmosphere by rainfall. Another compound with a relatively low  $\tau_{w,g}^{(V/P)}$  was mercuric chloride (HgCl<sub>2</sub>), with an estimated value of  $\sim 1.4$  days. Interestingly, mercury in precipitation has been found to be correlated with concentrations of chloride ion, suggesting that an important form of mercury in precipitation is HgCl<sub>2</sub> (Keeler, Glinsorn, and Pirrono, 1995).

Of course, rainfall is a sporadic event, and a given "air parcel" may not encounter a rain event for days or weeks. Thus, this very short characteristic time for rain removal does not guarantee that MBOCA will not be transported for long distances in the atmosphere. Rather, it suggests that wet deposition of gas phase material will be a very effective removal process, and the "average" atmospheric lifetime will depend on the frequency with which emitted material encounters a rain event.

Hamrud and Rodhe (1986) have estimated lagrangian time scales related to clouds and precipitation using a trajectory air transport model. They estimate that the average time a lagrangian air parcel exists in the atmosphere after being emitted before encountering its first cloud is on the order of a week, with variations around the world and in different seasons (the range is approximately from 0.5 - 2.5 weeks). Not all clouds produce rain, however, and so the average time to a rain event will be somewhat longer. Thus, the minimum average atmospheric lifetime for compounds relative to wet deposition -- even if they are very effectively removed by rain -- will be on the order of a week.

Figure D.1.-(1). Qualitative Assessment of the Time Scale for Gas Phase Washout by Wet Deposition from the Atmosphere



"Chem Layer Hght" = Height of Atmospheric Layer Within Which Chemical Assumed to be Evenly Mixed  
Rainfall Rate assumed to be 30 inches per year (0.0021 m/day)

Char. Time for Gas Phase Wet Dep. Removal from Atm.						
NAME			characteristic	for gas-phase	assume precipitation rate of 30"/yr	
			time for gas phase	wet dep divided	assume chemical mixing layer depth of 5000 meters	
			wet deposition	by avg frac	assume temperature = 290 degrees K	
			of compound	in gas phase	assume mid-range value of average fraction in gas phase	
common chemical name	IUPAC #	cas # (1)	[=] days	[=] days	notes	
octachlorostyrene	029082-74-4		1.3E+004	1.3E+004		
4-bromophenyl phenyl ether	000101-55-3		1.0E+004	1.0E+004		
3,3'-dichlorobenzidine	000091-94-1		5.0E+000	4.8E+001		
1,3-dinitropyrene	075321-20-9		5.7E+001	8.7E+001	crude estm of H; uncertainty in this characteristic time at least +/- a factor of 10	
1,6-dinitropyrene	042397-64-8		5.7E+001	8.7E+001	crude estm of H; uncertainty in this characteristic time at least +/- a factor of 10	
1,8-dinitropyrene	042397-65-9		5.7E+001	8.7E+001	crude estm of H; uncertainty in this characteristic time at least +/- a factor of 10	
2,7-dinitropyrene	117929-15-4		5.7E+001	8.7E+001	crude estm of H; uncertainty in this characteristic time at least +/- a factor of 10	
dinitropyrenes (mixed)	078432-19-6					
hexachloro-1,3-butadiene	000087-68-3		1.5E+006	1.5E+006		
4,4'-methylene bis(2-chloroaniline)	000101-14-4		4.0E-003	4.1E-003		
pentachlorophenol	000087-86-5		7.8E+001	7.9E+001	will depend on pH of rain; will be less soluble in more acidic rain.	
aldrin	000309-00-2		5.0E+004	5.0E+004		
dieleadrin	000060-57-1		5.8E+003	5.9E+003		
p,p'-DDT	000050-29-3		5.2E+004	7.2E+004		
p,p'-DDD	000072-54-8		2.2E+003	2.4E+003		
p,p'-DDE	000072-55-9		6.8E+003	7.0E+003		
heptachlor	000076-44-8		1.5E+005	1.5E+005		
heptachlor epoxide	001024-57-3		3.2E+003	3.2E+003		
methoxychlor	000072-43-5		1.6E+003	1.8E+003		
mirex	002385-85-5		8.3E+005	8.3E+005		
toxaphene	008001-35-2		6.0E+002	6.7E+002		
endrin	000072-20-8		7.6E+002	7.6E+002		
alpha-hexachlorocyclohexane	000319-84-6		5.4E+002	5.4E+002		
beta-hexachlorocyclohexane	000319-85-7		4.5E+001	4.5E+001		
delta-hexachlorocyclohexane	000319-86-8		2.1E+001	2.1E+001		
gamma-hexachlorocyclohexane	000058-89-9		5.5E+002	5.6E+002		
mixed hexachlorocyclohexanes	000319-84-6					

Char. Time for Gas Phase Wet Dep. Removal from Atm.						
NAME			characteristic	for gas-phase	assume precipitation rate of 30"/yr	
			time for	wet dep	assume chemical mixing layer depth of 5000 meters	
			gas phase	divided	assume temperature = 290 degrees K	
			wet deposition	by avg frac	assume mid-range value of average fraction in gas phase	
			of compound	in gas phase		
common chemical name	IUPAC #	cas # (1)	[=] days	[=] days	notes	
cadmium	007440-43-9					
cadmium carbonate	000513-78-0					
cadmium chloride	010108-64-2					
cadmium oxide	001306-19-0					
cadmium sulfate	010124-36-4					
cadmium sulfide	001306-23-6					
elemental mercury	007439-97-6		5.7E+005	5.7E+005		
mercury oxide	021908-53-2					
mercuric chloride	007487-94-7		1.4E+000	1.4E+000		
monomethyl mercury chloride	000115-09-3					
dimethyl mercury	000593-74-8					
tetraethyl lead	000078-00-2		5.7E+007	5.7E+007		
tetramethyl lead	000075-74-1		8.8E+007	8.8E+007		
triethyl lead radical (1+ cation)	014570-15-1					
triethyl lead hydride	005224-23-7					
triethyl lead chloride	001067-14-7					
diethyl lead radical (2+ cation)	024952-65-6					
diethyl lead dihydride	081494-11-3					
diethyl lead dichloride	013231-90-8					
trimethyl lead radical (1+ cation)	014570-16-2					
trimethyl lead hydride	007442-13-9					
trimethyl lead chloride	001520-78-1					
dimethyl lead radical (2+ cation)	021774-13-0					
dimethyl lead dihydride	030691-92-0					
dimethyl lead dichloride	001520-77-0					
bis (tributyltin) oxide	000056-35-9		1.3E+001	2.4E+001		
tributyl tin	000688-75-3					
tributyltin fluoride	001983-10-4					
tributyltin chloride	001461-22-9					
tributyltin hydroxide	001067-97-6					
tributyltin naphthenate						
tris(tributylstannyl) phosphate	013435-05-7					

Char. Time for Gas Phase Wet Dep. Removal from Atm.						
NAME				characteristic time for gas phase wet deposition of compound	for gas-phase wet dep divided by avg frac in gas phase	assume precipitation rate of 30"/yr assume chemcal mixing layer depth of 5000 meters assume temperature = 290 degrees K assume mid-range value of average fraction in gas phase
common chemical name	IUPAC #	cas # (1)		[=] days	[=] days	notes
1,4-dichlorobenzene	000106-46-7			1.6E+005	1.6E+005	
1,2,3,4-tetrachlorobenzene	000634-66-2			1.4E+005	1.4E+005	
1,2,4,5-tetrachlorobenzene	000095-94-3			1.2E+005	1.2E+005	
1,2,3,5-tetrachlorobenzene	000634-90-2			5.8E+005	5.8E+005	
pentachlorobenzene	000608-93-5			8.4E+004	8.4E+004	
hexachlorobenzene	000118-74-1			1.3E+005	1.3E+005	
naphthalene	000091-20-3			4.3E+004	4.3E+004	
acenaphthene	000083-32-9			1.2E+004	1.2E+004	
acenaphthylene	000208-96-8			8.3E+003	8.3E+003	
fluorene	000086-73-7			7.8E+003	7.8E+003	
phenanthrene	000085-01-8			3.2E+003	3.2E+003	
anthracene	000120-12-7			3.9E+003	3.9E+003	
pyrene	000129-00-0			9.1E+002	9.2E+002	
fluoranthene	000206-44-0			1.0E+003	1.0E+003	
chrysene	000218-01-9			1.1E+002	1.9E+002	
benz [ a ] anthracene	000056-55-3			5.8E+002	1.2E+003	
benzo [ b ] fluoranthene	000205-99-2			1.2E+003	1.3E+003	
benzo [ j ] fluoranthene	000205-82-3			1.0E+002	2.9E+002	
benzo [ k ] fluoranthene	000207-08-9			1.6E+001	3.6E+002	
benzo [ a ] pyrene	000050-32-8			4.6E+001	2.5E+002	
benzo [ e ] pyrene	000192-97-2			2.0E+001	1.0E+002	
perylene	000198-55-0			3.0E+000	6.3E+001	
benzo [ g,h,i ] perylene	000191-24-2			7.4E+001	1.7E+003	
dibenz [ a,h ] anthracene	000053-70-3			7.3E+000	7.3E+003	
indeno [ 1,2,3-c,d ] pyrene	000193-39-5			7.0E+000	1.3E+003	

Char. Time for Gas Phase Wet Dep. Removal from Atm.								
NAME								
			characteristic		for gas-phase		assume precipitation rate of 30"/yr	
			time for		wet dep		assume chemical mixing layer depth of 5000 meters	
			gas phase		divided		assume temperature = 290 degrees K	
			wet deposition		by avg frac		assume mid-range value of average fraction in gas phase	
			of compound		in gas phase			
common chemical name	IUPAC #	cas # (1)	[=] days	[=] days			notes	
2,3,7,8-TCDD	001746-01-6		3.3E+003	8.0E+003				
1,2,3,7,8-PeCDD	040321-76-4		2.6E+002	5.9E+003				
1,2,3,4,7,8-HxCDD	039227-28-6		1.1E+003	6.6E+004				
1,2,3,6,7,8-HxCDD	057653-85-7		1.1E+003	6.6E+004				
1,2,3,7,8,9-HxCDD	019408-74-3		1.1E+003	6.6E+004				
1,2,3,4,6,7,8-HpCDD	035822-46-9		1.3E+003	6.4E+005				
OCDD	003268-87-9		6.8E+002	6.2E+005				
2,3,7,8-TCDF	051207-31-9		1.5E+003	2.1E+003				
2,3,4,7,8-PeCDF	057117-31-4		5.0E+002	3.1E+003				
1,2,3,7,8-PeCDF	057117-41-6		5.0E+002	3.1E+003				
1,2,3,4,7,8-HxCDF	070648-26-9		1.4E+003	4.4E+004				
1,2,3,6,7,8-HxCDF	057117-44-9		7.4E+002	1.8E+004				
1,2,3,7,8,9-HxCDF	072918-21-9		1.1E+003	2.9E+004				
2,3,4,6,7,8-HxCDF	060851-34-5		1.1E+003	2.9E+004				
1,2,3,4,6,7,8-HpCDF	067562-39-4		1.4E+003	2.3E+005				
1,2,3,4,7,8,9-HpCDF	055673-89-7		1.4E+003	2.4E+005				
OCDF	039001-02-0		1.9E+002	1.7E+005				

Char. Time for Gas Phase Wet Dep. Removal from Atm.						
NAME						
				char. time	assume precipitation rate of 30"/yr	
				characteristic	for gas-phase	assume chemical mixing layer depth of 5000 meters
				time for	wet dep	assume temperature = 290 degrees K
				gas phase	divided	assume mid-range value of average fraction in gas phase
				wet deposition	by avg frac	
				of compound	in gas phase	
common chemical name	IUPAC #	cas # (1)	[=] days	[=] days	notes	
biphenyl	0	000092-52-4	5.3E+004	5.3E+004		
2-PCB	1	002051-60-7	7.0E+004	7.0E+004		
3-PCB	2	002051-61-8	7.5E+004	7.5E+004		
4-PCB	3	002051-62-9	4.2E+004	4.2E+004		
count						
average						
standard deviation						
minimum						
maximum						
2,2'-PCB	4	013029-08-8	5.9E+004	5.9E+004		
2,3-PCB	5	016605-91-7				
2,4-PCB	7	033284-50-3	4.5E+004	4.5E+004		
2,4'-PCB	8	034883-43-7				
2,5-PCB	9	034883-39-1	2.0E+004	2.0E+004		
2,6-PCB	10	033146-45-1				
3,3'-PCB	11	002050-67-1	1.7E+004	1.7E+004		
3,4-PCB	12	002974-92-7				
3,5-PCB	14	034883-41-5				
4,4'-PCB	15	002050-68-2	1.7E+004	1.7E+004		
count						
average						
standard deviation						
minimum						
maximum						

Char. Time for Gas Phase Wet Dep. Removal from Atm.						
NAME				characteristic	char. time	assume precipitation rate of 30"/yr assume chemical mixing layer depth of 5000 meters assume temperature = 290 degrees K assume mid-range value of average fraction in gas phase
					for gas-phase	
					time for gas phase	
common chemical name	IUPAC #	cas # (1)	[=] days	wet deposition	by avg frac	assume temperature = 290 degrees K assume mid-range value of average fraction in gas phase
				of compound	in gas phase	
2,2',3-PCB	16	038444-78-9				
2,2',5-PCB	18	037680-65-2	9.2E+004		9.2E+004	
2,3,3'-PCB	20	038444-84-7				
2,3,4-PCB	21	055702-46-0				
2,3',5-PCB	26	038444-85-8				
2,4,4'-PCB	28	007012-37-5				
2,4,5-PCB	29	015862-07-4	2.4E+004		2.4E+004	
2,4,6-PCB	30	035693-92-6	4.9E+004		4.9E+004	
2,4,5,-PCB	31	016606-02-3				
2',3,4-PCB	33	038444-86-9	4.3E+004		4.4E+004	
3,3',4-PCB	35	037680-69-6				
3,4,4'-PCB	37	038444-90-5				
count						
average						
standard deviation						
minimum						
maximum						
2,2,3,3'-PCB	40	038444-93-8	2.2E+004		2.2E+004	
2,2',3,5'-PCB	44	041464-39-5				
2,2',4,4'-PCB	47	002437-79-8	1.7E+004		1.7E+004	
2,2',4,5'-PCB	49	041464-40-8				
2,2',4,6-PCB	50	062796-65-0				
2,2',4,6'-PCB	51	068194-04-7				
2,2,5,5'-PCB	52	035693-99-3	4.7E+004		4.8E+004	
2,2,5,6'-PCB	53	041464-41-9				
2,2,6,6'-PCB	54	015968-05-5				
2,3,4,4'-PCB	60	033025-41-1				
2,3,4,5-PCB	61	033284-53-6				
2,3,5,6-PCB	65	033284-54-7				
2,3,4,4'-PCB	66	032598-10-0				
2,3',4',5-PCB	70	032598-11-1				
2,4,4',6-PCB	75	032598-12-2				
3,3',4,4'-PCB	77	032598-13-3	1.7E+003		1.8E+003	
3,3',5,5'-PCB	80	033284-52-5				
3,4,4',5-PCB	81	070362-50-4				
count						
average						
standard deviation						
minimum						
maximum						

Char. Time for Gas Phase Wet Dep. Removal from Atm.						
NAME			characteristic	for gas-phase	assume precipitation rate of 30"/yr	
			time for gas phase	wet dep divided	assume chemical mixing layer depth of 5000 meters	
			wet deposition	by avg frac of compound	assume temperature = 290 degrees K	
				in gas phase	assume mid-range value of average fraction in gas phase	
common chemical name	IUPAC #	cas # (1)	[=] days	[=] days	notes	
2,2',3,3',5-PCB	83	060145-20-2				
2,2',3,4,5-PCB	86	065510-45-4	1.5E+005	1.6E+005		
2,2',3,4,5'-PCB	87	038380-02-8	2.5E+004	2.6E+004		
2,2',3,4,6-PCB	88	055215-17-3				
2,2',3,5,6-PCB	95	038379-99-6				
2,2',4,4',5-PCB	99	038380-01-7				
2,2',4,4',6-PCB	100	039485-83-1				
2,2',4,5,5'-PCB	101	037680-73-2	3.5E+004	3.7E+004		
2,2',4,6,6'-PCB	104	056558-16-8	1.4E+004	1.5E+004		
2,3,3',4,4'-PCB	105	032598-14-4				
2,3,3',4,6-PCB	110	038380-03-9				
2,3,4,4',5-PCB	114	074472-37-0				
2,3,4,5,6-PCB	116	018259-05-7				
2,3,4,4',5-PCB	118	031508-00-6				
2,3,4,5,5'-PCB	124	070424-70-3				
3,3',4,4',5-PCB	126	057465-28-8				
count						
average						
standard deviation						
minimum						
maximum						
2,2',3,3',4,4'-PCB	128	038380-07-3	1.2E+004	1.8E+004		
2,2',3,3',4,5-PCB	129	055215-18-4				
2,2',3,3',5,6-PCB	134	052704-70-8				
2,2',3,3',6,6'-PCB	136	038411-22-2				
2,2',3,4,4',5-PCB	138	035065-28-2				
2,2',3,4',5,6-PCB	149	038380-04-0				
2,2',4,4',5,5'-PCB	153	035065-27-1	4.3E+004	5.3E+004		
2,2',4,4',6,6'-PCB	155	033979-03-2	8.6E+004	8.9E+004		
2,3,3',4,4',5-PCB	156	038380-08-4				
2,3,3',4,4',5'-PCB	157	069782-90-7				
2,3,3',4,4',5,5'-PCB	167	052663-72-6				
3,3',4,4',5,5'-PCB	169	032774-16-6				
count						
average						
standard deviation						
minimum						
maximum						

Char. Time for Gas Phase Wet Dep. Removal from Atm.						
NAME			characteristic	for gas-phase	assume precipitation rate of 30"/yr	
			time for gas phase	wet dep divided	assume chemical mixing layer depth of 5000 meters	
			wet deposition	by avg frac	assume temperature = 290 degrees K	
			of compound	in gas phase	assume mid-range value of average fraction in gas phase	
common chemical name	IUPAC #	cas # (1)	[=] days	[=] days	notes	
2,2',3,3',4,4',5-PCB	170	035065-30-6				
2,2',3,3',4,4',6-PCB	171	052663-71-5	5.4E+003	1.0E+004		
2,2',3,4,4',5,5'-PCB	180	035065-29-3				
2,2',3,4,5,5',6-PCB	185	052712-05-7				
2,2',3,4',5,5'-PCB	187	052663-68-0				
2,3,3',4,4',5,5'-PCB	189	039635-31-9				
count						
average						
standard deviation						
minimum						
maximum						
2,2',3,3',4,4',5,5'-PCB	194	035694-08-7				
2,2',3,3',5,5',6,6'-PCB	202	002136-99-4	3.8E+004	5.0E+004		
count						
average						
standard deviation						
minimum						
maximum						
2,2',3,3',4,4',5,5',6-PCB	206	040186-72-9	8.2E+004	1.6E+006		
2,2',3,3',4,4',5,6,6'-PCB	207	052663-79-3				
2,2',3,3',4,5,5',6,6'-PCB	208	052663-77-1				
count						
average						
standard deviation						
minimum						
maximum						
2,2',3,3',4,4',5,5',6,6'-PCB	209	002051-24-3	2.1E+004	3.1E+005		

## **Appendix D.2.**

**Basic Results for Gas Phase Reaction Rate with Hydroxyl Radical  
(limited data on reactions with O<sub>3</sub> and NO<sub>3</sub> also summarized)**

MDC	MDC	ESTM RXN RATE with HYDROXYL RADICAL		Atm Half Life				EXPT'L: RXN RATE with OH		
		AOPWIN	AOPWIN	AOPWIN	MDC	AOPWIN	AOPWIN	AOPWIN	AOPWIN	AOPWIN
		AOPWIN output text indicating that it tried to estim OH rxn	AOPWIN estimated an OH Rate rxn rate of with Hydroxyl Estimate 12 for this	estimated Reaction half-life (days) assuming hours/day and [OH]= 1.5E+006 cm3/	estimated Reaction half-life (days) assuming hours/day and [OH]= 1.5E+006 cm3/	AOPWIN output text indicating that it tried to find expt'l OH	AOPWIN output text indicating that it tried to find expt'l OH	EXPT'L: RXN RATE with OH cm3/(molecule-sec)		
octachlorostyrene		(OH est)		1.07311E-012	9.968	---(exp OH)	0			
4-bromophenyl phenyl ether		(OH est)		6.33066E-012	1.690	---(exp OH)	0			
3,3'-dichlorobenzidine		(OH est)		3.95704E-011	0.270	---(exp OH)	0			
1,3-dinitropyrene		(OH est)		5.46000E-013	19.591	---(exp OH)	0			
1,6-dinitropyrene		(OH est)		5.46000E-013	19.591	---(exp OH)	0			
1,8-dinitropyrene		(OH est)		5.46000E-013	19.591	---(exp OH)	0			
2,7-dinitropyrene		(OH est)		5.46000E-013	19.591	---(exp OH)	0			
dinitropyrenes (mixed)							0			
hexachloro-1,3-butadiene		(OH est)		3.00200E-014	356.320	---(exp OH)	0			
4,4'-methylene bis(2-chloroaniline)		(OH est)		7.75166E-011	0.138	---(exp OH)	0			
pentachlorophenol		(OH est)		5.50490E-013	19.431	---(exp OH)	0			
aldrin		(OH est)		6.45895E-011	0.166	---(exp OH)	0			
diechlorodrin		(OH est)		8.83921E-012	1.210	---(exp OH)	0			
p,p'-DDT		(OH est)		3.43505E-012	3.114	---(exp OH)	0			
p,p'-DDD		(OH est)		4.34415E-012	2.462	---(exp OH)	0			
p,p'-DDE		(OH est)		7.43011E-012	1.440	---(exp OH)	0			
heptachlor		(OH est)		6.13278E-011	0.174	---(exp OH)	0			
heptachlor epoxide		(OH est)		3.84870E-012	2.779	---(exp OH)	0			
methoxychlor		(OH est)		5.35478E-011	0.200	---(exp OH)	0			
mirex		(OH est)	0.00E+000			---(exp OH)	0			
toxaphene		(OH est)		2.49555E-012	4.286	---(exp OH)	0			
endrin		(OH est)		8.83921E-012	1.210	---(exp OH)	0			
alpha-hexachlorocyclohexane		(OH est)		5.73250E-013	18.660	---(exp OH)	0			
beta-hexachlorocyclohexane		(OH est)		5.73250E-013	18.660	---(exp OH)	0			
delta-hexachlorocyclohexane		(OH est)		5.73250E-013	18.660	---(exp OH)	0			
gamma-hexachlorocyclohexane		(OH est)		5.73250E-013	18.660	---(exp OH)	0			
mixed hexachlorocyclohexanes		(OH est)		5.73250E-013	18.660	---(exp OH)	0			
cadmium							0			
cadmium carbonate							0			
cadmium chloride		(OH est)	0.00E+000			---(exp OH)	0			
cadmium oxide		(OH est)	0.00E+000			---(exp OH)	0			
cadmium sulfate							0			
cadmium sulfide		(OH est)	0.00E+000			---(exp OH)	0			
elemental mercury							0			
mercury oxide		(OH est)	0.00E+000			---(exp OH)	0			
mercuric chloride		(OH est)	0.00E+000			---(exp OH)	0			
monomethyl mercury chloride		(OH est)		8.16000E-012	1.311	---(exp OH)	0			
dimethyl mercury		(OH est)		1.63200E-011	0.655	---(exp OH)	1	1.90E-011		

MDC	MDC	ESTM RXN RATE with HYDROXYL RADICAL		Atm Half Life				EXPT'L: RXN RATE with OH		
		AOPWIN	AOPWIN	AOPWIN	MDC	AOPWIN	AOPWIN	AOPWIN	AOPWIN	AOPWIN
		AOPWIN output text indicating that it tried to estim OH rxn	AOPWIN estimated an OH Rate Estimate with Hydroxyl rxn rate for this	estimated Reaction Rate 12 hours/day and [OH]= 1.5E+006 cm3/	estimated half-life (days) assuming 12 hours/day that it tried and [OH]= 1.5E+006 expt'l OH	AOPWIN output text indicating that it tried to find OH	EXPT'L: RXN RATE with OH cm3/(molecule-sec)	AVG Expt'l OH	LOW Expt'l OH	HIGH Expt'l OH
tetraethyl lead		(OH est)		4.92371E-011	0.217	----(exp OH)	1	6.00E-011		
tetramethyl lead		(OH est)		7.07200E-012	1.513	----(exp OH)	1	6.00E-012		
triethyl lead radical (1+ cation)		(OH est)		3.69278E-011	0.290	----(exp OH)	0			
triethyl lead hydride		(OH est)		3.69278E-011	0.290	----(exp OH)	0			
triethyl lead chloride		(OH est)		3.69278E-011	0.290	----(exp OH)	0			
diethyl lead radical (2+ cation)		(OH est)		2.46186E-011	0.434	----(exp OH)	0			
diethyl lead dihydride		(OH est)		2.46186E-011	0.434	----(exp OH)	0			
diethyl lead dichloride		(OH est)		2.46186E-011	0.434	----(exp OH)	0			
trimethyl lead radical (1+ cation)		(OH est)		5.30400E-012	2.017	----(exp OH)	0			
trimethyl lead hydride		(OH est)		5.30400E-012	2.017	----(exp OH)	0			
trimethyl lead chloride		(OH est)		5.30400E-012	2.017	----(exp OH)	0			
dimethyl lead radical (2+ cation)		(OH est)		3.53600E-012	3.025	----(exp OH)	0			
dimethyl lead dihydride							0			
dimethyl lead dichloride		(OH est)		3.53600E-012	3.025	----(exp OH)	0			
bis (tributyltin) oxide		(OH est)		8.53041E-011	0.125	----(exp OH)	0			
tributyl tin							0			
tributyltin fluoride		(OH est)		4.26520E-011	0.251	----(exp OH)	0			
tributyltin chloride		(OH est)		4.26520E-011	0.251	----(exp OH)	0			
tributyltin hydroxide		(OH est)		4.27920E-011	0.250	----(exp OH)	0			
tributyltin naphthenate							0			
tris(tributylstannyl) phosphate							0			
1,4-dichlorobenzene		(OH est)		4.00480E-013	26.710	----(exp OH)	1	3.20E-013		
1,2,3,4-tetrachlorobenzene		(OH est)		8.22500E-014	130.051	----(exp OH)	0			
1,2,4,5-tetrachlorobenzene		(OH est)		8.22500E-014	130.051	----(exp OH)	0			
1,2,3,5-tetrachlorobenzene		(OH est)		1.98180E-013	53.975	----(exp OH)	0			
pentachlorobenzene		(OH est)		5.78600E-014	184.872	----(exp OH)	0			
hexachlorobenzene		(OH est)		1.68900E-014	633.317	----(exp OH)	0			
naphthalene		(OH est)		2.16000E-011	0.495	----(exp OH)	1	2.16E-011		
acenaphthene		(OH est)		6.72285E-011	0.159	----(exp OH)	1	7.85E-011	5.40E-011	1.03E-010
acenaphthylene		(OH est)		7.54921E-011	0.142	----(exp OH)	1	1.10E-010		
fluorene		(OH est)		9.00093E-012	1.188	----(exp OH)	1	1.20E-011		
phenanthrene		(OH est)		1.30000E-011	0.823	----(exp OH)	1	1.30E-011		
anthracene		(OH est)		4.00000E-011	0.267	----(exp OH)	1	4.00E-011		
pyrene		(OH est)		5.00000E-011	0.214	----(exp OH)	1	5.00E-011		
fluoranthene		(OH est)		2.92273E-011	0.366	----(exp OH)	1	5.00E-011		
chrysene		(OH est)		5.00000E-011	0.214	----(exp OH)	0			
benz [ a ] anthracene		(OH est)		5.00000E-011	0.214	----(exp OH)	0			
benzo [ b ] fluoranthene		(OH est)		1.85540E-011	0.577	----(exp OH)	0			

MDC	MDC	ESTM RXN RATE with HYDROXYL RADICAL		Atm Half Life				EXPT'L: RXN RATE with OH			
		AOPWIN	AOPWIN	AOPWIN	MDC	AOPWIN	AOPWIN	AOPWIN	AOPWIN	AOPWIN	
		AOPWIN output text indicating that it tried to estim OH rxn	AOPWIN estimated an OH rxn rate of 0.0e-12 for this	AOPWIN estimated Reaction Rate Estimate with Hydroxyl 12 hours/day and [OH]= 1.5E+006 expt'l OH cm3/	estimated half-life (days) assuming 12 hours/day and [OH]= 1.5E+006 expt'l OH cm3/	AOPWIN output text indicating that it tried to find OH	EXPT'L: RXN RATE with OH cm3/(molecule-sec)	AVG Expt'l OH	LOW Expt'l OH	HIGH Expt'l OH	
benzo [ j ] fluoranthene		(OH est)		5.36147E-011	0.200	----(exp OH)	0				
benzo [ k ] fluoranthene		(OH est)		5.36147E-011	0.200	----(exp OH)	0				
benzo [ a ] pyrene		(OH est)		5.00000E-011	0.214	----(exp OH)	0				
benzo [ e ] pyrene		(OH est)		5.00000E-011	0.214	----(exp OH)	0				
perylene		(OH est)		5.00000E-011	0.214	----(exp OH)	0				
benzo [ g,h,i ] perylene		(OH est)		8.68620E-011	0.123	----(exp OH)	0				
dibenz [ a,h ] anthracene		(OH est)		5.00000E-011	0.214	----(exp OH)	0				
indeno [ 1,2,3-c,d ] pyrene		(OH est)		6.44740E-011	0.166	----(exp OH)	0				
2,3,7,8-TCDD		(OH est)		2.02120E-012	5.292	----(exp OH)	0				
1,2,3,7,8-PeCDD		(OH est)		1.72152E-012	6.214	----(exp OH)	0				
1,2,3,4,7,8-HxCDD		(OH est)		1.21817E-012	8.781	----(exp OH)	0				
1,2,3,6,7,8-HxCDD		(OH est)		1.42184E-012	7.523	----(exp OH)	0				
1,2,3,7,8,9-HxCDD		(OH est)		1.42184E-012	7.523	----(exp OH)	0				
1,2,3,4,6,7,8-HpCDD		(OH est)		9.18490E-013	11.646	----(exp OH)	0				
OCDD		(OH est)		4.15140E-013	25.767	----(exp OH)	0				
2,3,7,8-TCDF		(OH est)		1.64520E-013	65.018	----(exp OH)	0				
2,3,4,7,8-PeCDF		(OH est)		7.45600E-014	143.465	----(exp OH)	0				
1,2,3,7,8-PeCDF		(OH est)		7.45600E-014	143.465	----(exp OH)	0				
1,2,3,4,7,8-HxCDF		(OH est)		3.03550E-013	35.239	----(exp OH)	0				
1,2,3,6,7,8-HxCDF		(OH est)		3.58920E-013	29.803	----(exp OH)	0				
1,2,3,7,8,9-HxCDF		(OH est)		3.38000E-014	316.471	----(exp OH)	0				
2,3,4,6,7,8-HxCDF		(OH est)		3.03980E-013	35.189	----(exp OH)	0				
1,2,3,4,6,7,8-HpCDF		(OH est)		1.53100E-014	698.675	----(exp OH)	0				
1,2,3,4,7,8,9-HpCDF		(OH est)		1.53000E-014	699.132	----(exp OH)	0				
OCDF		(OH est)		6.94000E-015	1541.314	----(exp OH)	0				
biphenyl	0	(OH est)		6.77470E-012	1.579	----(exp OH)	1	7.20E-012			
2-PCB	1	(OH est)		3.48475E-012	3.070	----(exp OH)	1	2.82E-012			
3-PCB	2	(OH est)		4.87861E-012	2.193	----(exp OH)	1	5.28E-012			
4-PCB	3	(OH est)		3.48475E-012	3.070	----(exp OH)	1	3.86E-012			
2,2'-PCB	4	(OH est)		1.72691E-012	6.194	----(exp OH)	1	2.00E-012			
2,3-PCB	5	(OH est)		2.47319E-012	4.325	----(exp OH)	0				
2,4-PCB	7	(OH est)		2.46678E-012	4.336	----(exp OH)	1	2.60E-012			
2,4'-PCB	8	(OH est)		1.72691E-012	6.194	----(exp OH)	0				
2,5-PCB	9	(OH est)		2.47319E-012	4.325	----(exp OH)	0				
2,6-PCB	10	(OH est)		2.46678E-012	4.336	----(exp OH)	0				
3,3'-PCB	11	(OH est)		3.51132E-012	3.046	----(exp OH)	1	4.10E-012			
3,4-PCB	12	(OH est)		2.47319E-012	4.325	----(exp OH)	0				
3,5-PCB	14	(OH est)		3.45372E-012	3.097	----(exp OH)	1	4.20E-012			

MDC	MDC	ESTM RXN RATE with HYDROXYL RADICAL		Atm Half Life				EXPT'L: RXN RATE with OH		
		AOPWIN	AOPWIN	AOPWIN	MDC	AOPWIN	AOPWIN	AOPWIN	AOPWIN	AOPWIN
		AOPWIN output text indicating that it tried to estim OH rxn	AOPWIN estimated an OH Rate rxn rate Estimate of with Hydroxyl OH rxn for this	estimated Reaction Rate Estimate 12 hours/day and [OH]= 1.5E+006 expt'l OH cm3/	half-life (days) assuming 12 hours/day that it tried and [OH]= 1.5E+006 expt'l OH cm3/	AOPWIN output text indicating that it tried to find OH	EXPT'L: RXN RATE with OH cm3/(molecule-sec)	AVG Expt'l OH	LOW Expt'l OH	HIGH Expt'l OH
4,4'-PCB	15	(OH est)		1.72691E-012	6.194	----(exp OH)	1	2.00E-012		
2,2',3-PCB	16	(OH est)		1.09075E-012	9.807	----(exp OH)	0			
2,2',5-PCB	18	(OH est)		1.09075E-012	9.807	----(exp OH)	0			
2,3,3'-PCB	20	(OH est)		1.76298E-012	6.067	----(exp OH)	0			
2,3,4-PCB	21	(OH est)		1.25509E-012	8.523	----(exp OH)	0			
2,3',5-PCB	26	(OH est)		1.09075E-012	9.807	----(exp OH)	0			
2,4,4'-PCB	28	(OH est)		1.18556E-012	9.023	----(exp OH)	1	1.10E-012		
2,4,5-PCB	29	(OH est)		1.25509E-012	8.523	----(exp OH)	1	1.30E-012		
2,4,6-PCB	30	(OH est)		1.53687E-012	6.960	----(exp OH)	0			
2,4',5-PCB	31	(OH est)		1.09080E-012	9.806	----(exp OH)	1	1.20E-012		
2',3,4-PCB	33	(OH est)		1.09075E-012	9.807	----(exp OH)	1	1.00E-012		
3,3',4-PCB	35	(OH est)		1.76300E-012	6.067	----(exp OH)	0			
3,4,4'-PCB	37	(OH est)		1.09080E-012	9.806	----(exp OH)	0			
2,2',3,3'-PCB	40	(OH est)		7.30150E-013	14.650	----(exp OH)	0			
2,2',3,5'-PCB	44	(OH est)		7.30150E-013	14.650	----(exp OH)	1	8.00E-013		
2,2',4,4'-PCB	47	(OH est)		8.13400E-013	13.151	----(exp OH)	1	1.00E-012		
2,2',4,5'-PCB	49	(OH est)		7.71780E-013	13.860	----(exp OH)	0			
2,2',4,6-PCB	50	(OH est)		8.26530E-013	12.942	----(exp OH)	0			
2,2',4,6'-PCB	51	(OH est)		8.13410E-013	13.150	----(exp OH)	0			
2,2,5,5'-PCB	52	(OH est)		7.30150E-013	14.650	----(exp OH)	0			
2,2,5,6'-PCB	53	(OH est)		7.71780E-013	13.860	----(exp OH)	0			
2,2,6,6'-PCB	54	(OH est)		8.13410E-013	13.150	----(exp OH)	0			
2,3,4,4'-PCB	60	(OH est)		5.76590E-013	18.552	----(exp OH)	0			
2,3,4,5-PCB	61	(OH est)		8.05110E-013	13.286	----(exp OH)	0			
2,3,5,6-PCB	65	(OH est)		8.05110E-013	13.286	----(exp OH)	0			
2,3,4,4'-PCB	66	(OH est)		7.71780E-013	13.860	----(exp OH)	0			
2,3',4',5-PCB	70	(OH est)		7.30150E-013	14.650	----(exp OH)	0			
2,4,4',6-PCB	75	(OH est)		8.26530E-013	12.942	----(exp OH)	0			
3,3',4,4'-PCB	77	(OH est)		7.30150E-013	14.650	----(exp OH)	0			
3,3',5,5'-PCB	80	(OH est)		1.75918E-012	6.081	----(exp OH)	0			
3,4,4',5-PCB	81	(OH est)		7.59800E-013	14.078	----(exp OH)	0			
2,2',3,3',5-PCB	83	(OH est)		4.72900E-013	22.619	----(exp OH)	0			
2,2',3,4,5-PCB	86	(OH est)		3.99600E-013	26.769	----(exp OH)	0			
2,2',3,4,5'-PCB	87	(OH est)		3.34810E-013	31.949	----(exp OH)	0			
2,2',3,4,6-PCB	88	(OH est)		4.18010E-013	25.590	----(exp OH)	0			
2,2',3,5,6-PCB	95	(OH est)		3.34810E-013	31.949	----(exp OH)	1	4.00E-013		
2,2',4,4',5-PCB	99	(OH est)		3.99600E-013	26.769	----(exp OH)	0			
2,2',4,4',6-PCB	100	(OH est)		5.66950E-013	18.867	----(exp OH)	0			

MDC	MDC	ESTM RXN RATE with HYDROXYL RADICAL		Atm Half Life				EXPT'L: RXN RATE with OH			
		AOPWIN	AOPWIN	AOPWIN	MDC	AOPWIN	AOPWIN	AOPWIN	AOPWIN	AOPWIN	
		AOPWIN output text indicating that it tried to estim OH rxn	AOPWIN estimated an OH rxn rate Estimate of with Hydroxyl 12 hours/day and [OH]= 1.5E+006 rxn OH for this cm3/	estimated Reaction Rate Estimate with Hydroxyl 12 hours/day and [OH]= 1.5E+006 expt'l OH	AOPWIN half-life (days) assuming text	EXPT'L: RXN RATE with OH cm3/(molecule-sec)					
2,2',4,5,5'-PCB	101	(OH est)		3.34810E-013	31.949	----(exp OH)	0				
2,2',4,6,6'-PCB	104	(OH est)		5.66950E-013	18.867	----(exp OH)	0				
2,3,3',4,4'-PCB	105	(OH est)		3.34810E-013	31.949	----(exp OH)	0				
2,3,3',4,6-PCB	110	(OH est)		3.34810E-013	31.949	----(exp OH)	1	6.00E-013			
2,3,4,4',5-PCB	114	(OH est)		3.98530E-013	26.840	----(exp OH)	0				
2,3,4,5,6-PCB	116	(OH est)		5.28130E-013	20.254	----(exp OH)	1	9.00E-013			
2,3,4,4',5-PCB	118	(OH est)		3.34810E-013	31.949	----(exp OH)	0				
2',3,4,5,5'-PCB	124	(OH est)		4.72880E-013	22.620	----(exp OH)	0				
3,3',4,4',5-PCB	126	(OH est)		4.72900E-013	22.619	----(exp OH)	0				
2,2',3,3',4,4'-PCB	128	(OH est)		1.64000E-013	65.224	----(exp OH)	0				
2,2',3,3',4,5-PCB	129	(OH est)		2.11000E-013	50.695	----(exp OH)	0				
2,2',3,3',5,6-PCB	134	(OH est)		2.11000E-013	50.695	----(exp OH)	0				
2,2',3,3',6,6'-PCB	136	(OH est)		1.64000E-013	65.224	----(exp OH)	0				
2,2',3,4,4',5-PCB	138	(OH est)		1.64000E-013	65.224	----(exp OH)	0				
2,2',3,4',5,6-PCB	149	(OH est)		1.64000E-013	65.224	----(exp OH)	0				
2,2',4,4',5,5'-PCB	153	(OH est)		1.64000E-013	65.224	----(exp OH)	0				
2,2',4,4',6,6'-PCB	155	(OH est)		3.95140E-013	27.071	----(exp OH)	0				
2,3,3',4,4',5-PCB	156	(OH est)		2.11000E-013	50.695	----(exp OH)	0				
2,3,3',4,4',5'-PCB	157	(OH est)		2.34000E-013	45.712	----(exp OH)	0				
2,3,4,4',5,5'-PCB	167	(OH est)		2.33990E-013	45.714	----(exp OH)	0				
3,3',4,4',5,5'-PCB	169	(OH est)		3.03980E-013	35.189	----(exp OH)	0				
2,2',3,3',4,4',5-PCB	170	(OH est)		1.04610E-013	102.253	----(exp OH)	0				
2,2',3,3',4,4',6-PCB	171	(OH est)		1.17920E-013	90.712	----(exp OH)	0				
2,2',3,4,4',5,5'-PCB	180	(OH est)		1.04610E-013	102.253	----(exp OH)	0				
2,2',3,4,5,5',6-PCB	185	(OH est)		1.24290E-013	86.063	----(exp OH)	0				
2,2',3,4',5,5',6-PCB	187	(OH est)		1.04610E-013	102.253	----(exp OH)	0				
2,3,3',4,4',5,5'-PCB	189	(OH est)		1.40060E-013	76.372	----(exp OH)	0				
2,2',3,3',4,4',5,5'-PCB	194	(OH est)		5.58700E-014	191.457	----(exp OH)	0				
2,2',3,3',5,5',6,6'-PCB	202	(OH est)		5.58700E-014	191.457	----(exp OH)	0				
2,2',3,3',4,4',5,5',6-PCB	206	(OH est)		3.28900E-014	325.227	----(exp OH)	0				
2,2',3,3',4,4',5,6,6'-PCB	207	(OH est)		4.34900E-014	245.958	----(exp OH)	0				
2,2',3,3',4,5,5',6,6'-PCB	208	(OH est)		3.28900E-014	325.227	----(exp OH)	0				
2,2',3,3',4,4',5,5',6,6'-PCB	209	(OH est)		1.81700E-014	588.702	----(exp OH)	0				

Chemical Name	IUPAC #	CAS #	ozone?	rxn with molec.-sec	estimated rxn rate cm3/ molec.sec	estimated half-life (days)	estimated half-life (days)	EXPT'L: RXN RATE with O3			EXPT'L: RXN RATE with NO3		
								cm3/(molecule-sec)			cm3/(molecule-sec)		
								exist?	<?	Value	exist?	<?	Value
octachlorostyrene		029082-74-4		1	6.14E-020	186.619	187	0			0		
4-bromophenyl phenyl ether		000101-55-3		0				0			0		
3,3'-dichlorobenzidine		000091-94-1		0				0			0		
1,3-dinitropyrene		075321-20-9		0				0			0		
1,6-dinitropyrene		042397-64-8		0				0			0		
1,8-dinitropyrene		042397-65-9		0				0			0		
2,7-dinitropyrene		117929-15-4		0				0			0		
dinitropyrenes (mixed)		078432-19-6		0				0			0		
hexachloro-1,3-butadiene		000087-68-3	1	7.00E-023		163,725	0				0		
4,4'-methylene bis(2-chloroaniline)		000101-14-4		0				0			0		
pentachlorophenol		000087-86-5		0				0			0		
aldrin		000309-00-2	1	2.00E-016		0.057	0				0		
dieleadrin		000060-57-1	1	3.58E-020		320	0				0		
p,p'-DDT		000050-29-3		0				0			0		
p,p'-DDD		000072-54-8		0				0			0		
p,p'-DDE		000072-55-9	1	5.15E-018		2.2	0				0		
heptachlor		000076-44-8	1	2.00E-016		0.057	0				0		
heptachlor epoxide		001024-57-3	1	3.58E-020		320	0				0		
methoxychlor		000072-43-5		0				0			0		
mirex		002385-85-5		0				0			0		
toxaphene		008001-35-2		0				0			0		
endrin		000072-20-8	1	3.58E-020		320	0				0		
alpha-hexachlorocyclohexane		000319-84-6		0				0			0		
beta-hexachlorocyclohexane		000319-85-7		0				0			0		
delta-hexachlorocyclohexane		000319-86-8		0				0			0		
gamma-hexachlorocyclohexane		000058-89-9		0				0			0		
mixed hexachlorocyclohexanes		000319-84-6		0				0			0		
cadmium		007440-43-9		0				0			0		
cadmium carbonate		000513-78-0		0				0			0		
cadmium chloride		010108-64-2		0				0			0		
cadmium oxide		001306-19-0		0				0			0		
cadmium sulfate		010124-36-4		0				0			0		
cadmium sulfide		001306-23-6		0				0			0		
elemental mercury		007439-97-6		0				0			0		
mercury oxide		021908-53-2		0				0			0		
mercuric chloride		007487-94-7		0				0			0		
monomethyl mercury chloride		000115-09-3		0				0			0		
dimethyl mercury		000593-74-8		0				0			0		
tetraethyl lead		000078-00-2		0				0			0		
tetramethyl lead		000075-74-1		0				0			0		
triethyl lead radical (1+ cation)		014570-15-1		0				0			0		
triethyl lead hydride		005224-23-7		0				0			0		
triethyl lead chloride		001067-14-7		0				0			0		
diethyl lead radical (2+ cation)		024952-65-6		0				0			0		
diethyl lead dihydride		081494-11-3		0				0			0		
diethyl lead dichloride		013231-90-8		0				0			0		
trimethyl lead radical (1+ cation)		014570-16-2		0				0			0		
trimethyl lead hydride		007442-13-9		0				0			0		
trimethyl lead chloride		001520-78-1		0				0			0		
dimethyl lead radical (2+ cation)		021774-13-0		0				0			0		
dimethyl lead dihydride		030691-92-0		0				0			0		
dimethyl lead dichloride		001520-77-0		0				0			0		

Chemical Name	IUPAC #	CAS #	estimated half-life (days) did rxn rate with ozone?	estimated half-life (days) hours/day rxn with ozone? and [O3]= cm3/ molec.-sec	estimated half-life (days) hours/day and [O3]= cm3/ molec/cm3	exist? <?	EXPT'L: RXN RATE with O3 cm3/(molecule-sec)			EXPT'L: RXN RATE with NO3 cm3/(molecule-sec)		
							AVG	LOW	HIGH	AVG	LOW	HIGH
							Expt'l	Expt'l	Expt'l	O3	O3	O3
bis (tributyltin) oxide		000056-35-9	0		0					0		
tributyl tin		000688-75-3	0		0					0		
tributyltin fluoride		001983-10-4	0		0					0		
tributyltin chloride		001461-22-9	0		0					0		
tributyltin hydroxide		001067-97-6	0		0					0		
tributyltin naphthenate			0		0					0		
tris(tributylstannyl) phosphate		013435-05-7	0		0					0		
1,4-dichlorobenzene		000106-46-7	0		0					0		
1,2,3,4-tetrachlorobenzene		000634-66-2	0		0					0		
1,2,4,5-tetrachlorobenzene		000095-94-3	0		0					0		
1,2,3,5-tetrachlorobenzene		000634-90-2	0		0					0		
pentachlorobenzene		000608-93-5	0		0					0		
hexachlorobenzene		000118-74-1	0		0					0		
naphthalene		000091-20-3	0		1 < 2E-019					1	6.4E-015	
acenaphthene		000083-32-9	0		0					0		
acenaphthylene		000208-96-8	1	2.52E-016	0.045					0		
fluorene		000086-73-7	0		0					0		
phenanthrene		000085-01-8	0		0					0		
anthracene		000120-12-7	0		0					0		
pyrene		000129-00-0	0		0					0		
fluoranthene		000206-44-0	0		0					0		
chrysene		000218-01-9	0		0					0		
benz [ a ] anthracene		000056-55-3	0		0					0		
benzo [ b ] fluoranthene		000205-99-2	0		0					0		
benzo [ j ] fluoranthene		000205-82-3	0		0					0		
benzo [ k ] fluoranthene		000207-08-9	0		0					0		
benzo [ a ] pyrene		000050-32-8	0		0					0		
benzo [ e ] pyrene		000192-97-2	0		0					0		
perylene		000198-55-0	0		0					0		
benzo [ g,h,i ] perylene		000191-24-2	0		0					0		
dibenz [ a,h ] anthracene		000053-70-3	0		0					0		
indeno [ 1,2,3-c,d ] pyrene		000193-39-5	0		0					0		
2,3,7,8-TCDD		001746-01-6	0		0					0		
1,2,3,7,8-PeCDD		040321-76-4	0		0					0		
1,2,3,4,7,8-HxCDD		039227-28-6	0		0					0		
1,2,3,6,7,8-HxCDD		057653-85-7	0		0					0		
1,2,3,7,8,9-HxCDD		019408-74-3	0		0					0		
1,2,3,4,6,7,8-HpCDD		035822-46-9	0		0					0		
OCDD		003268-87-9	0		0					0		
2,3,7,8-TCDF		051207-31-9	0		0					0		
2,3,4,7,8-PeCDF		057117-31-4	0		0					0		
1,2,3,7,8-PeCDF		057117-41-6	0		0					0		
1,2,3,4,7,8-HxCDF		070648-26-9	0		0					0		
1,2,3,6,7,8-HxCDF		057117-44-9	0		0					0		
1,2,3,7,8,9-HxCDF		072918-21-9	0		0					0		
2,3,4,6,7,8-HxCDF		060851-34-5	0		0					0		
1,2,3,4,6,7,8-HpCDF		067562-39-4	0		0					0		
1,2,3,4,7,8,9-HpCDF		055673-89-7	0		0					0		
OCDF		039001-02-0	0		0					0		
biphenyl	0	000092-52-4	0		1 < *****					0		
2-PCB	1	002051-60-7	0		0					0		
3-PCB	2	002051-61-8	0		0					0		

Chemical Name	IUPAC #	CAS #	estimated half-life (days)	estimated half-life (days)	EXPT'L: RXN RATE with O3						EXPT'L: RXN RATE with NO3							
					AOPWIN with ozone			hours/day			cm3/(molecule-sec)			O3			cm3/(molecule-sec)	
			Best estimate	rxn with ozone?	cm3/	molec.-sec	molec/cm3	molec/cm3	exist?	<?	Value	Value	Value	exist?	<?	Value	Value	Value
4-PCB	3	002051-62-9	0						0					0				
2,2'-PCB	4	013029-08-8	0						0					0				
2,3-PCB	5	016605-91-7	0						0					0				
2,4-PCB	7	033284-50-3	0						0					0				
2,4'-PCB	8	034883-43-7	0						0					0				
2,5-PCB	9	034883-39-1	0						0					0				
2,6-PCB	10	033146-45-1	0						0					0				
3,3'-PCB	11	002050-67-1	0						0					0				
3,4-PCB	12	002974-92-7	0						0					0				
3,5-PCB	14	034883-41-5	0						0					0				
4,4'-PCB	15	002050-68-2	0						0					0				
2,2,3-PCB	16	038444-78-9	0						0					0				
2,2,5-PCB	18	037680-65-2	0						0					0				
2,3,3'-PCB	20	038444-84-7	0						0					0				
2,3,4-PCB	21	055702-46-0	0						0					0				
2,3,5-PCB	26	038444-85-8	0						0					0				
2,4,4'-PCB	28	007012-37-5	0						0					0				
2,4,5-PCB	29	015862-07-4	0						0					0				
2,4,6-PCB	30	035693-92-6	0						0					0				
2,4',5,-PCB	31	016606-02-3	0						0					0				
2,3,4-PCB	33	038444-86-9	0						0					0				
3,3',4-PCB	35	037680-69-6	0						0					0				
3,4,4'-PCB	37	038444-90-5	0						0					0				
2,2',3,3'-PCB	40	038444-93-8	0						0					0				
2,2',3,5'-PCB	44	041464-39-5	0						0					0				
2,2',4,4'-PCB	47	002437-79-8	0						0					0				
2,2',4,5'-PCB	49	041464-40-8	0						0					0				
2,2,4,6-PCB	50	062796-65-0	0						0					0				
2,2',4,6'-PCB	51	068194-04-7	0						0					0				
2,2,5,5'-PCB	52	035693-99-3	0						0					0				
2,2,5,6'-PCB	53	041464-41-9	0						0					0				
2,2,6,6'-PCB	54	015968-05-5	0						0					0				
2,3,4,4'-PCB	60	033025-41-1	0						0					0				
2,3,4,5-PCB	61	033284-53-6	0						0					0				
2,3,5,6-PCB	65	033284-54-7	0						0					0				
2,3,4,4'-PCB	66	032598-10-0	0						0					0				
2,3',4',5-PCB	70	032598-11-1	0						0					0				
2,4,4',6-PCB	75	032598-12-2	0						0					0				
3,3',4,4'-PCB	77	032598-13-3	0						0					0				
3,3,5,5'-PCB	80	033284-52-5	0						0					0				
3,4,4',5-PCB	81	070362-50-4	0						0					0				
2,2',3,3',5-PCB	83	060145-20-2	0						0					0				
2,2',3,4,5-PCB	86	065510-45-4	0						0					0				
2,2',3,4,5'-PCB	87	038380-02-8	0						0					0				
2,2,3,4,6-PCB	88	055215-17-3	0						0					0				
2,2',3,5,6-PCB	95	038379-99-6	0						0					0				
2,2',4,4',5-PCB	99	038380-01-7	0						0					0				
2,2',4,4',6-PCB	100	039485-83-1	0						0					0				
2,2,4,5,5'-PCB	101	037680-73-2	0						0					0				
2,2,4,6,6'-PCB	104	056558-16-8	0						0					0				
2,3,3',4,4'-PCB	105	032598-14-4	0						0					0				
2,3,3',4,6-PCB	110	038380-03-9	0						0					0				

Chemical Name	IUPAC #	CAS #	estimated half-life (days)	estimated rxn rate with ozone and [O <sub>3</sub> ]= cm3/ molec.-sec	estimated half-life (days) assuming rxn with cm3/ molec/cm3	exist? <?	EXPT'L: RXN RATE with O <sub>3</sub> cm3/(molecule-sec)			EXPT'L: RXN RATE with NO <sub>3</sub> cm3/(molecule-sec)		
							AVG	LOW	HIGH	AVG	LOW	HIGH
							Expt'l	Expt'l	Expt'l	O <sub>3</sub>	O <sub>3</sub>	O <sub>3</sub>
2,3,4,4',5-PCB	114	074472-37-0	0		0					0		
2,3,4,5,6-PCB	116	018259-05-7	0		0					0		
2,3',4,4',5-PCB	118	031508-00-6	0		0					0		
2,3,4,5,5'-PCB	124	070424-70-3	0		0					0		
3,3',4,4',5-PCB	126	057465-28-8	0		0					0		
2,2,3,3',4,4'-PCB	128	038380-07-3	0		0					0		
2,2,3,3',4,5-PCB	129	055215-18-4	0		0					0		
2,2',3,3',5,6-PCB	134	052704-70-8	0		0					0		
2,2',3,3',6,6'-PCB	136	038411-22-2	0		0					0		
2,2',3,4,4',5-PCB	138	035065-28-2	0		0					0		
2,2,3,4,5,6-PCB	149	038380-04-0	0		0					0		
2,2',4,4',5,5'-PCB	153	035065-27-1	0		0					0		
2,2,4,4',6,6'-PCB	155	033979-03-2	0		0					0		
2,3,3',4,4',5-PCB	156	038380-08-4	0		0					0		
2,3,3',4,4',5-PCB	157	069782-90-7	0		0					0		
2,3,4,4',5,5'-PCB	167	052663-72-6	0		0					0		
3,3',4,4',5,5'-PCB	169	032774-16-6	0		0					0		
2,2,3,3',4,4',5-PCB	170	035065-30-6	0		0					0		
2,2,3,3',4,4',6-PCB	171	052663-71-5	0		0					0		
2,2',3,4,4',5,5'-PCB	180	035065-29-3	0		0					0		
2,2,3,4,5,5,6-PCB	185	052712-05-7	0		0					0		
2,2',3,4,5,5,6-PCB	187	052663-68-0	0		0					0		
2,3,3,4,4',5,5'-PCB	189	039635-31-9	0		0					0		
2,2,3,3',4,4',5,5'-PCB	194	035694-08-7	0		0					0		
2,2',3,3',5,5,6,6'-PCB	202	002136-99-4	0		0					0		
2,2',3,3',4,4',5,5,6-PCB	206	040186-72-9	0		0					0		
2,2',3,3',4,4',5,6,6'-PCB	207	052663-79-3	0		0					0		
2,2,3,3',4,5,5,6,6'-PCB	208	052663-77-1	0		0					0		
2,2',3,3',4,4',5,5,6,6'-PCB	209	002051-24-3	0		0					0		

### **Appendix D.3.**

#### **Atmospheric Lifetime Relative to Gas Phase Reaction Rates, Adjusted for Vapor Particle Partitioning**

ATMOSPHERIC HALFLIFE RELATIVE to RXN with OH (with some data for rxn with O3 also included)							
NAME	IUPAC #	cas # (1)	(molec.-sec)	Reaction Rate (days) assuming OH Estimate with Hydroxyl cm3/ molecule-sec	estm OH 1/2-life (days) assuming rxn rate	estm O3 1/2-life (days) assuming half-life	mimumum (rxn w OH or O3) divided by fraction in gas phase (days)
common chemical name							
octachlorostyrene	029082-74-4			1.07E-012	9.968	6.14E-020	186.657
4-bromophenyl phenyl ether	000101-55-3			6.33E-012	1.690		1.691
3,3'-dichlorobenzidine	000091-94-1			3.96E-011	0.270		2.618
1,3-dinitropyrene	075321-20-9			5.46E-013	19.591		30.086
1,6-dinitropyrene	042397-64-8			5.46E-013	19.591		30.086
1,8-dinitropyrene	042397-65-9			5.46E-013	19.591		30.086
2,7-dinitropyrene	117929-15-4			5.46E-013	19.591		30.086
dinitropyrenes (mixed)	078432-19-6						
hexachloro-1,3-butadiene	000087-68-3			3.00E-014	356.320	7.00E-023	163725.241
4,4'-methylene bis(2-chloroaniline)	000101-14-4			7.75E-011	0.138		0.139
pentachlorophenol	000087-86-5			5.50E-013	19.431		19.444
aldrin	000309-00-2			6.46E-011	0.166	2.00E-016	0.057
dieldrin	000060-57-1			8.84E-012	1.210	3.58E-020	320.223
p,p'-DDT	000050-29-3			3.44E-012	3.114		4.371
p,p'-DDD	000072-54-8			4.34E-012	2.462		2.699
p,p'-DDE	000072-55-9			7.43E-012	1.440	5.15E-018	2.224
heptachlor	000076-44-8			6.13E-011	0.174	2.00E-016	0.057
heptachlor epoxide	001024-57-3			3.85E-012	2.779	3.58E-020	320.223
methoxychlor	000072-43-5			5.35E-011	0.200		0.221
mirex	002385-85-5						
toxaphene	008001-35-2			2.50E-012	4.286		4.790
endrin	000072-20-8			8.84E-012	1.210	3.58E-020	320.223
alpha-hexachlorocyclohexane	000319-84-6			5.73E-013	18.660		18.671
beta-hexachlorocyclohexane	000319-85-7			5.73E-013	18.660		18.689
delta-hexachlorocyclohexane	000319-86-8			5.73E-013	18.660		18.682
gamma-hexachlorocyclohexane	000058-89-9			5.73E-013	18.660		18.713
mixed hexachlorocyclohexanes	000319-84-6			5.73E-013	18.660		18.660

ATMOSPHERIC HALFLIFE RELATIVE to RXN with OH (with some data for rxn with O3 also included)								
NAME	IUPAC #	cas # (1)	(molec.-sec)	AVG Expt'l OH Value cm3/	Reaction Rate Estimate with Hydroxyl cm3/ molecule-sec)	estm OH 1/2-life (days) assuming and [OH]= 1.5E+006	estm O3 1/2-life (days) assuming and [O3]= 7.0E+011	mimumum half-life hours/day with ozone and [O3]= gas phase divided by hours/day fraction in (rxn w OH or O3) (days)
common chemical name								
cadmium	007440-43-9							
cadmium carbonate	000513-78-0							
cadmium chloride	010108-64-2							
cadmium oxide	001306-19-0							
cadmium sulfate	010124-36-4							
cadmium sulfide	001306-23-6							
elemental mercury	007439-97-6							
mercury oxide	021908-53-2							
mercuric chloride	007487-94-7							
monomethyl mercury chloride	000115-09-3			8.16E-012	1.311		1.311	
dimethyl mercury	000593-74-8			1.90E-011	1.63E-011	0.655		0.655
tetraethyl lead	000078-00-2			6.00E-011	4.92E-011	0.217		0.217
tetramethyl lead	000075-74-1			6.00E-012	7.07E-012	1.513		1.513
triethyl lead radical (1+ cation)	014570-15-1			3.69E-011	0.290			
triethyl lead hydride	005224-23-7			3.69E-011	0.290			
triethyl lead chloride	001067-14-7			3.69E-011	0.290			
diethyl lead radical (2+ cation)	024952-65-6			2.46E-011	0.434			
diethyl lead dihydride	081494-11-3			2.46E-011	0.434			
diethyl lead dichloride	013231-90-8			2.46E-011	0.434			
trimethyl lead radical (1+ cation)	014570-16-2			5.30E-012	2.017			
trimethyl lead hydride	007442-13-9			5.30E-012	2.017			
trimethyl lead chloride	001520-78-1			5.30E-012	2.017			
dimethyl lead radical (2+ cation)	021774-13-0			3.54E-012	3.025			
dimethyl lead dihydride	030691-92-0							
dimethyl lead dichloride	001520-77-0			3.54E-012	3.025			
bis (tributyltin) oxide	000056-35-9			8.53E-011	0.125		0.239	
tributyl tin	000688-75-3							
tributyltin fluoride	001983-10-4			4.27E-011	0.251			
tributyltin chloride	001461-22-9			4.27E-011	0.251			
tributyltin hydroxide	001067-97-6			4.28E-011	0.250			
tributyltin naphthenate								
tris(tributylstanny) phosphate	013435-05-7							

ATMOSPHERIC HALFLIFE RELATIVE to RXN with OH (with some data for rxn with O3 also included)								
NAME			AVG	Reaction	estm OH 1/2-life	estm O3 1/2-life	mimumum	
			Expt'l	Rate	(days) assuming	estimated	(days) assuming	half-life
			OH	Estimate	12	rxn rate	24	(rxn w OH or O3)
			Value	with Hydroxyl	hours/day	with ozone	hours/day	divided by
					and [OH]=		and [O3]=	fraction in
					cm3/	cm3/	7.0E+011	gas phase
common chemical name	IUPAC #	cas # (1)	(molec.-sec)	(molecule-sec)	molecules/cm3	molec.-sec	molecules/cm3	(days)
1,4-dichlorobenzene	000106-46-7	3.20E-013	4.00E-013	26.710			26.710	
1,2,3,4-tetrachlorobenzene	000634-66-2		8.23E-014	130.051			130.052	
1,2,4,5-tetrachlorobenzene	000095-94-3		8.23E-014	130.051			130.052	
1,2,3,5-tetrachlorobenzene	000634-90-2		1.98E-013	53.975			53.975	
pentachlorobenzene	000608-93-5		5.79E-014	184.872			184.889	
hexachlorobenzene	000118-74-1		1.69E-014	633.317			633.516	
naphthalene	000091-20-3	2.16E-011	2.16E-011	0.495			0.495	
acenaphthene	000083-32-9	7.85E-011	6.72E-011	0.159			0.159	
acenaphthylene	000208-96-8	1.10E-010	7.55E-011	0.142	2.52E-016	0.045	0.045	
fluorene	000086-73-7	1.20E-011	9.00E-012	1.188			1.189	
phenanthrene	000085-01-8	1.30E-011	1.30E-011	0.823			0.823	
anthracene	000120-12-7	4.00E-011	4.00E-011	0.267			0.268	
pyrene	000129-00-0	5.00E-011	5.00E-011	0.214			0.215	
fluoranthene	000206-44-0	5.00E-011	2.92E-011	0.366			0.370	
chrysene	000218-01-9		5.00E-011	0.214			0.384	
benz [ a ] anthracene	000056-55-3		5.00E-011	0.214			0.432	
benzo [ b ] fluoranthene	000205-99-2		1.86E-011	0.577			0.608	
benzo [ j ] fluoranthene	000205-82-3		5.36E-011	0.200			0.575	
benzo [ k ] fluoranthene	000207-08-9		5.36E-011	0.200			4.573	
benzo [ a ] pyrene	000050-32-8		5.00E-011	0.214			1.158	
benzo [ e ] pyrene	000192-97-2		5.00E-011	0.214			1.101	
perylene	000198-55-0		5.00E-011	0.214			4.547	
benzo [ g,h,i ] perylene	000191-24-2		8.69E-011	0.123			2.802	
dibenz [ a,h ] anthracene	000053-70-3		5.00E-011	0.214			213.199	
indeno [ 1,2,3-c,d ] pyrene	000193-39-5		6.45E-011	0.166			31.840	

ATMOSPHERIC HALFLIFE RELATIVE to RXN with OH (with some data for rxn with O3 also included)							
NAME			AVG	Reaction	estm OH 1/2-life	estm O3 1/2-life	mimumum
			Expt'l	Rate	(days) assuming	estimated	half-life
			OH	Estimate	12	rxn rate	24 (rxn w OH or O3)
			Value	with Hydroxyl	hours/day	with ozone	hours/day divided by
					and [OH]=	and [O3]=	fraction in
				cm3/	cm3/	cm3/	gas phase
common chemical name	IUPAC #	cas # (1)	(molec.-sec)	(molecule-sec)	molecules/cm3	molec.-sec	molecules/cm3 (days)
2,3,7,8-TCDD	001746-01-6			2.02E-012	5.292		12.831
1,2,3,7,8-PeCDD	040321-76-4			1.72E-012	6.214		138.871
1,2,3,4,7,8-HxCDD	039227-28-6			1.22E-012	8.781		541.159
1,2,3,6,7,8-HxCDD	057653-85-7			1.42E-012	7.523		463.641
1,2,3,7,8,9-HxCDD	019408-74-3			1.42E-012	7.523		463.641
1,2,3,4,6,7,8-HpCDD	035822-46-9			9.18E-013	11.646		5910.600
OCDD	003268-87-9			4.15E-013	25.767		23515.495
2,3,7,8-TCDF	051207-31-9			1.65E-013	65.018		93.174
2,3,4,7,8-PeCDF	057117-31-4			7.46E-014	143.465		895.754
1,2,3,7,8-PeCDF	057117-41-6			7.46E-014	143.465		895.754
1,2,3,4,7,8-HxCDF	070648-26-9			3.04E-013	35.239		1070.669
1,2,3,6,7,8-HxCDF	057117-44-9			3.59E-013	29.803		717.409
1,2,3,7,8,9-HxCDF	072918-21-9			3.38E-014	316.471		8548.215
2,3,4,6,7,8-HxCDF	060851-34-5			3.04E-013	35.189		950.489
1,2,3,4,6,7,8-HpCDF	067562-39-4			1.53E-014	698.675		112057.229
1,2,3,4,7,8,9-HpCDF	055673-89-7			1.53E-014	699.132		120715.569
OCDF	039001-02-0			6.94E-015	1541.314		1420877.201

ATMOSPHERIC HALFLIFE RELATIVE to RXN with OH (with some data for rxn with O3 also included)							
NAME			AVG	Reaction	estm OH 1/2-life	estm O3 1/2-life	mimum
			Expt'l	Rate	(days) assuming	estimated	half-life
			OH	Estimate	12	rxn rate	24 (rxn w OH or O3)
			Value	with Hydroxyl	hours/day	with ozone	hours/day divided by
					and [OH]=	and [O3]=	fraction in
				cm3/	cm3/	cm3/	gas phase
common chemical name	IUPAC #	cas # (1)	(molec.-sec)	(molecule-sec)	molecules/cm3	molec.-sec	molecules/cm3 (days)
biphenyl	0	000092-52-4	7.20E-012	6.77E-012	1.579		1.579
2-PCB	1	002051-60-7	2.82E-012	3.48E-012	3.070		3.070
3-PCB	2	002051-61-8	5.28E-012	4.88E-012	2.193		2.193
4-PCB	3	002051-62-9	3.86E-012	3.48E-012	3.070		3.070
count				3	3		3
average				<b>3.95E-012</b>	<b>2.78E+000</b>		<b>2.78E+000</b>
standard deviation				6.57E-013	4.13E-001		4.13E-001
minimum				3.48E-012	2.19E+000		2.19E+000
maximum				4.88E-012	3.07E+000		3.07E+000
2,2'-PCB	4	013029-08-8	2.00E-012	1.73E-012	6.194		6.197
2,3-PCB	5	016605-91-7		2.47E-012	4.325		4.329
2,4-PCB	7	033284-50-3	2.60E-012	2.47E-012	4.336		4.340
2,4'-PCB	8	034883-43-7		1.73E-012	6.194		6.199
2,5-PCB	9	034883-39-1		2.47E-012	4.325		4.328
2,6-PCB	10	033146-45-1		2.47E-012	4.336		4.338
3,3'-PCB	11	002050-67-1	4.10E-012	3.51E-012	3.046		3.051
3,4-PCB	12	002974-92-7		2.47E-012	4.325		4.333
3,5-PCB	14	034883-41-5	4.20E-012	3.45E-012	3.097		3.101
4,4'-PCB	15	002050-68-2	2.00E-012	1.73E-012	6.194		6.206
count				10	10		10
average				<b>2.45E-012</b>	<b>4.64E+000</b>		<b>4.64E+000</b>
standard deviation				6.09E-013	1.12E+000		1.13E+000
minimum				1.73E-012	3.05E+000		3.05E+000
maximum				3.51E-012	6.19E+000		6.21E+000

ATMOSPHERIC HALFLIFE RELATIVE to RXN with OH (with some data for rxn with O3 also included)								
NAME			AVG	Reaction	estm OH 1/2-life	estm O3 1/2-life	mimum	
			Expt'l	Rate	(days) assuming	estimated	(days) assuming	half-life
			OH	Estimate	12	rxn rate	24	(rxn w OH or O3)
			Value	with Hydroxyl	hours/day	with ozone	hours/day	divided by
					and [OH]=		and [O3]=	fraction in
					cm3/	cm3/	7.0E+011	gas phase
common chemical name	IUPAC #	cas # (1)	(molec.-sec)	(molecule-sec)	molecules/cm3	molec.-sec	molecules/cm3	(days)
2,2',3-PCB	16	038444-78-9			1.09E-012	9.807		9.832
2,2',5-PCB	18	037680-65-2			1.09E-012	9.807		9.825
2,3,3'-PCB	20	038444-84-7			1.76E-012	6.067		6.099
2,3,4-PCB	21	055702-46-0			1.26E-012	8.523		8.568
2,3',5-PCB	26	038444-85-8			1.09E-012	9.807		9.842
2,4,4'-PCB	28	007012-37-5			1.10E-012	1.19E-012		9.061
2,4,5-PCB	29	015862-07-4			1.30E-012	1.26E-012		8.550
2,4,6-PCB	30	035693-92-6			1.54E-012	6.960		6.970
2,4',5-PCB	31	016606-02-3			1.20E-012	1.09E-012		9.858
2',3,4-PCB	33	038444-86-9			1.00E-012	1.09E-012		9.861
3,3',4-PCB	35	037680-69-6			1.76E-012	6.067		6.134
3,4,4'-PCB	37	038444-90-5			1.09E-012	9.806		9.924
count					12	12		12
average					1.28E-012	8.67E+000		8.71E+000
standard deviation					2.51E-013	1.43E+000		1.43E+000
minimum					1.09E-012	6.07E+000		6.10E+000
maximum					1.76E-012	9.81E+000		9.92E+000
2,2',3,3'-PCB	40	038444-93-8			7.30E-013	14.650		14.876
2,2',3,5-PCB	44	041464-39-5			8.00E-013	7.30E-013		14.823
2,2',4,4'-PCB	47	002437-79-8			1.00E-012	8.13E-013		13.280
2,2',4,5-PCB	49	041464-40-8				7.72E-013		13.984
2,2',4,6-PCB	50	062796-65-0				8.27E-013		13.514
2,2',4,6'-PCB	51	068194-04-7				8.13E-013		13.229
2,2,5,5'-PCB	52	035693-99-3				7.30E-013		14.787
2,2,5,6'-PCB	53	041464-41-9				7.72E-013		13.934
2,2,6,6'-PCB	54	015968-05-5				8.13E-013		13.197
2,3,4,4'-PCB	60	033025-41-1				5.77E-013		19.100
2,3,4,5-PCB	61	033284-53-6				8.05E-013		13.457
2,3,5,6-PCB	65	033284-54-7				8.05E-013		13.429
2,3,4,4'-PCB	66	032598-10-0				7.72E-013		14.205
2,3',4',5-PCB	70	032598-11-1				7.30E-013		15.072
2,4,4',6-PCB	75	032598-12-2				8.27E-013		13.050
3,3',4,4'-PCB	77	032598-13-3				7.30E-013		15.728
3,3',5,5'-PCB	80	033284-52-5				1.76E-012		6.262
3,4,4',5-PCB	81	070362-50-4				7.60E-013		14.880
count					18	18		18
average					8.20E-013	1.36E+001		1.39E+001
standard deviation					2.35E-013	2.22E+000		2.31E+000
minimum					5.77E-013	6.08E+000		6.26E+000
maximum					1.76E-012	1.86E+001		1.91E+001

ATMOSPHERIC HALFLIFE RELATIVE to RXN with OH (with some data for rxn with O3 also included)								
NAME			AVG	Reaction	estm OH 1/2-life	estm O3 1/2-life	mimum	
			Expt'l	Rate	(days) assuming	estimated	(days) assuming	half-life
			OH	Estimate	12	rxn rate	24	(rxn w OH or O3)
			Value	with Hydroxyl	hours/day	with ozone	hours/day	divided by
					and [OH]=		and [O3]=	fraction in
					cm3/	cm3/	7.0E+011	gas phase
common chemical name	IUPAC #	cas # (1)	(molec.-sec)	(molecule-sec)	molecules/cm3	molec.-sec	molecules/cm3	(days)
2,2',3,3',5-PCB	83	060145-20-2		4.73E-013	22.619		23.962	
2,2',3,4,5-PCB	86	065510-45-4		4.00E-013	26.769		28.321	
2,2',3,4,5'-PCB	87	038380-02-8		3.35E-013	31.949		34.217	
2,2',3,4,6-PCB	88	055215-17-3		4.18E-013	25.590		26.261	
2,2',3,5,6-PCB	95	038379-99-6	4.00E-013	3.35E-013	31.949		32.890	
2,2',4,4',5-PCB	99	038380-01-7		4.00E-013	26.769		28.210	
2,2',4,4',6-PCB	100	039485-83-1		5.67E-013	18.867		25.102	
2,2',4,5,5'-PCB	101	037680-73-2		3.35E-013	31.949		33.463	
2,2',4,6,6'-PCB	104	056558-16-8		5.67E-013	18.867		19.987	
2,3,3',4,4'-PCB	105	032598-14-4		3.35E-013	31.949		38.137	
2,3,3',4,6-PCB	110	038380-03-9	6.00E-013	3.35E-013	31.949		34.753	
2,3,4,4',5-PCB	114	074472-37-0		3.99E-013	26.840		30.426	
2,3,4,5,6-PCB	116	018259-05-7	9.00E-013	5.28E-013	20.254		21.666	
2,3',4,4',5-PCB	118	031508-00-6		3.35E-013	31.949		36.389	
2',3,4,5,5'-PCB	124	070424-70-3		4.73E-013	22.620		27.409	
3,3',4,4',5-PCB	126	057465-28-8		4.73E-013	22.619		30.830	
count				16	16		16	
average				4.19E-013	2.65E+001		2.95E+001	
standard deviation				8.22E-014	4.87E+000		5.13E+000	
minimum				3.35E-013	1.89E+001		2.00E+001	
maximum				5.67E-013	3.19E+001		3.81E+001	
2,2',3,3',4,4'-PCB	128	038380-07-3		1.64E-013	65.224		98.009	
2,2',3,3',4,5-PCB	129	055215-18-4		2.11E-013	50.695		70.288	
2,2',3,3',5,6-PCB	134	052704-70-8		2.11E-013	50.695		57.559	
2,2',3,3',6,6'-PCB	136	038411-22-2		1.64E-013	65.224		71.571	
2,2',3,4,4',5-PCB	138	035065-28-2		1.64E-013	65.224		86.919	
2,2',3,4',5,6-PCB	149	038380-04-0		1.64E-013	65.224		74.853	
2,2',4,4',5,5'-PCB	153	035065-27-1		1.64E-013	65.224		81.448	
2,2',4,4',6,6'-PCB	155	033979-03-2		3.95E-013	27.071		28.144	
2,3,3',4,4',5-PCB	156	038380-08-4		2.11E-013	50.695		91.501	
2,3,3',4,4',5'-PCB	157	069782-90-7		2.34E-013	45.712		86.540	
2,3',4,4',5,5'-PCB	167	052663-72-6		2.34E-013	45.714		74.620	
3,3',4,4',5,5'-PCB	169	032774-16-6		3.04E-013	35.189		136.891	
count				12	12		12	
average				2.18E-013	5.27E+001		7.99E+001	
standard deviation				6.71E-014	1.24E+001		2.45E+001	
minimum				1.64E-013	2.71E+001		2.81E+001	
maximum				3.95E-013	6.52E+001		1.37E+002	

ATMOSPHERIC HALFLIFE RELATIVE to RXN with OH (with some data for rxn with O3 also included)							
NAME			AVG	Reaction	estm OH 1/2-life	estm O3 1/2-life	mimum
			Expt'l	Rate	(days) assuming	estimated	half-life
			OH	Estimate	12	rxn rate	24 (rxn w OH or O3)
			Value	with Hydroxyl	hours/day	with ozone	hours/day divided by
					and [OH]=	and [O3]=	fraction in
					cm3/	cm3/	gas phase
common chemical name	IUPAC #	cas # (1)	(molec.-sec)	(molecule-sec)	molecules/cm3	molec.-sec	molecules/cm3 (days)
2,2',3,3',4,4',5-PCB	170	035065-30-6		1.05E-013	102.253		321.332
2,2',3,3',4,4',6-PCB	171	052663-71-5		1.18E-013	90.712		177.181
2,2',3,4,4',5,5'-PCB	180	035065-29-3		1.05E-013	102.253		242.250
2,2',3,4,5,5',6-PCB	185	052712-05-7		1.24E-013	86.063		133.420
2,2',3,4,5,5',6-PCB	187	052663-68-0		1.05E-013	102.253		160.382
2,3,3',4,4',5,5'-PCB	189	039635-31-9		1.40E-013	76.372		377.695
count				6	6		6
average				<b>1.16E-013</b>	<b>9.33E+001</b>		<b>2.35E+002</b>
standard deviation				1.32E-014	9.88E+000		8.86E+001
minimum				1.05E-013	7.64E+001		1.33E+002
maximum				1.40E-013	1.02E+002		3.78E+002
2,2',3,3',4,4',5,5'-PCB	194	035694-08-7		5.59E-014	191.457		2010.704
2,2',3,3',5,5',6,6'-PCB	202	002136-99-4		5.59E-014	191.457		254.537
count				2	2		2
average				<b>5.59E-014</b>	<b>1.91E+002</b>		<b>1.13E+003</b>
standard deviation				0.00E+000	0.00E+000		8.78E+002
minimum				5.59E-014	1.91E+002		2.55E+002
maximum				5.59E-014	1.91E+002		2.01E+003
2,2',3,3',4,4',5,5',6-PCB	206	040186-72-9		3.29E-014	325.227		6317.514
2,2',3,3',4,4',5,6,6'-PCB	207	052663-79-3		4.35E-014	245.958		1659.813
2,2',3,3',4,5,5',6,6'-PCB	208	052663-77-1		3.29E-014	325.227		2282.857
count				3	3		3
average				<b>3.64E-014</b>	<b>2.99E+002</b>		<b>3.42E+003</b>
standard deviation				5.00E-015	3.74E+001		2.06E+003
minimum				3.29E-014	2.46E+002		1.66E+003
maximum				4.35E-014	3.25E+002		6.32E+003
2,2',3,3',4,4',5,5',6,6'-PCB	209	002051-24-3		1.82E-014	588.702		8674.359

## Appendix D.4.

### Information about Atmospheric Photolysis (i.e., Destruction by UV Light)

<b>Table D.4.-(1). Some Information about Atmospheric Photolysis (i.e., Destruction by UV Light) for Compounds Considered in this Study</b>			
Chemical or Group	LVL	Estimated Fraction Adsorbed to Particles in Atm. (App. C) (1)	Information Regarding Atmospheric Photolysis All Information Imported Directly from ATSDR Toxicological Profiles (CD ROM version) unless otherwise indicated; References cited are as cited in the original (e.g. ATSDR) document. Time constraints did not allow the inclusion of these references in the bibliography for this report.
<b>METALS / ORGANOMETALLICS</b>			
Alkylated Lead TEL = Tetraethyl Lead TML = Tetramethyl Lead	I	<b>0.000002</b> (TEL) (0.00000007 - 0.00004)	
		<b>0.00000003</b> (TML) (1e-9 - 0.00004)	
Mercury	I	<b>0.0005</b> (Hg) (0.00001 - 0.02)	The main atmospheric transformation process for organomercurials appears to be photolysis (EPA 1984b; Johnson and Bramen 1974; Williston 1968).
		<b>0.0000004</b> (HgCl <sub>2</sub> ) (0.00000003 - 0.000003)	
		<b>0.000003</b> (HgCH <sub>3</sub> Cl) (0.0000002 - 0.00004)	
Cadmium	II	<b>1</b> (Cd) (0.8 - 1)	
		<b>1</b> (CdCl <sub>2</sub> )	
Tributyltin TBTO = Tributyltin Oxide	II	<b>0.5</b> (TBTO) (0.02 - 0.98)	<p>[in water:] Tributyltin has been shown to undergo slow photolysis (Maguire et al. 1983). The half-life of the photolysis reaction was estimated to be greater than 89 days. The direct photolysis of tributyltin in water initiates a sequential removal of the butyl groups, leading to inorganic tin as a residual. The reaction was much faster in the presence of fulvic acid (a major component of soil organic matter).</p> <p>The overall half-life of tributyltin (photolysis and biodegradation) in water was estimated to be on the order of months in Canadian lakes. However, the half-life of tributyltin in river waters in Georgia was estimated to be between 3 and 13 days (Lee et al. 1989). The degradation of the chemical was attributed to microalgae whereas direct photolysis did not appear to be important.</p>

**Table D.4.-(1). Some Information about Atmospheric Photolysis  
(i.e., Destruction by UV Light) for Compounds Considered in this Study**

Chemical or Group	LVL	Estimated Fraction Adsorbed to Particles in Atm. (App. C) (1)	Information Regarding Atmospheric Photolysis All Information Imported Directly from ATSDR Toxicological Profiles (CD ROM version) unless otherwise indicated; References cited are as cited in the original (e.g. ATSDR) document. Time constraints did not allow the inclusion of these references in the bibliography for this report.
<b>ORGANOCHLORINE BIOCIDES</b>			
Aldrin / Dieldrin	1	<b>0.0009</b> (Aldrin) (0.00004 - 0.02)	<p>While the evidence supports the view that a considerable proportion of the aldrin and dieldrin used in agriculture reaches the atmosphere, it seems probable that atmospheric degradation prevents accumulation of aldrin.</p> <p>In laboratory studies, aldrin is photochemically isomerized and epoxidized by sunlight to photoaldrin, dieldrin, or photodieldrin (Glotfelter 1978).</p> <p>Irradiation of aldrin (5 mg) vapor with ultraviolet light for 45 hours resulted in the formation of photoaldrin (20-30 mg) and dieldrin (50-60 mg).</p> <p>[IN WATER:]</p> <p>Aldrin, irradiated with ultraviolet light in an oxygenated aqueous solution, underwent little change except in the presence of amino acids and humic acids present in natural waters (Ross and Crosby 1975, 1985).</p> <p>In filtered natural field water, aldrin was photooxidized by 75% to dieldrin after 48 hours of irradiation at 238 nm (Ross and Crosby 1985).</p>
		<b>0.003</b> (Dieldrin) (0.0002 - 0.03)	<p>Irradiation of either photoaldrin (2 mg) or dieldrin (0.5 mg) vapor for 65 hours and 91 minutes, respectively, resulted in a single photoproduct, photodieldrin (20-30 mg), which was resistant to further photolyses (Crosby and Moilanen 1974).</p> <p><b>Since photodieldrin no longer contains a chromophore</b>, it is believed to be a stable photoproduct of aldrin (dieldrin) (Glotfelter 1978).</p> <p>However, results of a laboratory study showed that photolysis of photoaldrin and photodieldrin in the presence of triethylamine gave photometabolites arising from the loss of chlorine atoms (Dureja et al. 1986).</p> <p>Information regarding the persistence of photodieldrin in the atmosphere was not located; however, air samples taken in 1973 in Ireland contained dieldrin, but neither aldrin nor the photoproducts of aldrin or dieldrin were detected (Baldwin et al. 1977).</p> <p>The estimated lifetime of dieldrin in the atmosphere, based on reactions with atmospheric hydroxyl radicals, is approximately 1 day.</p> <p>However, dieldrin may be more stable than implied by this lifetime if it is associated with particulate matter in the atmosphere. Under these conditions, wet and dry deposition may be more important loss processes (Bidleman et al. 1990).</p> <p>[IN WATER:] More than 80% of the initial dieldrin added to natural water (from a drainage canal in an agricultural area) was present after 16 weeks of incubation in the dark (Sharon et al. 1980). Dieldrin exposed to sunlight is converted to photodieldrin, a stereoisomer of dieldrin. It is unlikely that photodieldrin occurs widely in the environment. Microorganisms isolated from lake water and lake-bottom sediments may convert dieldrin to photodieldrin under anaerobic conditions (Fries 1972).</p> <p>Dieldrin has been found to undergo minor degradation to photodieldrin in marine environments. The marine algae of the genus Dunaliella had the maximum degradation activity, degrading 23% of aldrin to dieldrin and 8.5% of dieldrin to photodieldrin (Patil et al. 1972).</p>

**Table D.4.-(1). Some Information about Atmospheric Photolysis  
(i.e., Destruction by UV Light) for Compounds Considered in this Study**

Chemical or Group	LVL	Estimated Fraction Adsorbed to Particles in Atm. (App. C) (1)	Information Regarding Atmospheric Photolysis All Information Imported Directly from ATSDR Toxicological Profiles (CD ROM version) unless otherwise indicated; References cited are as cited in the original (e.g. ATSDR) document. Time constraints did not allow the inclusion of these references in the bibliography for this report.
DDT / DDD / DDE	I	0.3 (DDT) (0.03 - 0.8)	<p>Environmental processes contribute to the degradation and transformation of DDT to different extents.</p> <p>Under simulated atmospheric conditions, both DDT and DDE decompose to form carbon dioxide and hydrochloric acid (WHO 1979).</p> <p><b>In air and sunlight, DDT is subject to direct photooxidation and reaction with photochemically produced hydroxyl radicals. The latter process has an estimated half-life of 2 days.</b></p> <p><b>Since DDT residues are ubiquitous in the atmosphere, it seems likely that photodegradation must occur at a slower rate than this estimated half-life.</b></p>
		0.09 (DDD) (0.005 - 0.6)	<p>DDT which reaches the photochemically active ionosphere may be rapidly destroyed by solar irradiation as indicated under laboratory conditions (Coulston 1985).</p> <p><b>IN WATER:</b></p> <p>DDT present in water may be converted by both photodegradation and biodegradation.</p>
		0.02 (DDE) (0.001 - 0.3)	<p><b>DDE in water absorbs short-wavelength ultraviolet sunlight (&lt;320 nm) and undergoes rapid photolysis. The photolysis half-life of DDE ranges from 0.94 to 6.1 days depending on the season.</b> DDE also undergoes photoisomerization when exposed to sunlight.</p> <p>Photolysis of DDE photoisomers is slower by at least one order of magnitude compared to DDE (Coulston 1985; Zepp et al. 1977).</p> <p>Biodegradation of DDT by aquatic microorganisms is reported to be a minor mechanism of transformation (Johnsen 1976).</p>

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Mirex	I	<b>0.00002</b> (0.000001 - 0.0005)	<p>Little information was found on the degradation of mirex in the atmosphere.</p> <p>Mirex is expected to be stable against photogenerated hydroxyl radicals in the atmosphere (Eisenreich et al. 1981).</p> <p><b>(Photolysis of chlordcone in the atmosphere does not appear to be an important degradation pathway for this compound); While nonvolatile products of photolysis were not monitored, only 1.8% of the chlordcone adsorbed on silica gel and exposed to ultraviolet light (wavelength &gt;290 nm) was photolyzed to carbon dioxide or other volatile compounds (Freitag et al. 1985).</b></p> <p>5.3.2.2 Water</p> <p><b>The degradation of mirex in water occurs primarily by photolysis.</b> During the photodecomposition of mirex, the chlorine atoms are replaced by hydrogen atoms.</p> <p>The primary photoreduction product of mirex in water is photomirex (Andrade et al. 1975); the rate of this reaction can be increased by the presence of dissolved organic matter (such as humic acids) and was greatest at 265 nm in Lake Ontario water (Mudambi and Hassett 1988).</p> <p>In Lake Ontario, Mudambi et al. (1992) reported that the ratio of photomirex to mirex (P/M) increased in the stratified surface layer of the lake from spring until autumn and in water from Oswego Harbor. P/M ratios in the mirex source sediments (the Niagara and Oswego Rivers) were very low (&lt;0.07), whereas higher P/M ratios were seen in the lake bottom sediments (&gt;0.10) and surface waters (&gt;0.30).</p> <p>These findings suggest that photomirex in Lake Ontario is produced by photolysis of mirex present in the surface waters and it is then partitioned between water, sediment, and biota.</p>

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Toxaphene	I	0.1 (0.004 - 0.8)	<p>5.3.2.1 Air</p> <p><b>Direct photolytic degradation of toxaphene in the troposphere apparently does not occur.</b></p> <p>No information was found regarding the susceptibility of toxaphene to free radical oxidation in the atmosphere.</p> <p>The worldwide, long-range atmospheric transport of the mixture suggests that toxaphene is relatively resistant to transformation in the atmosphere.</p> <p>Since the production of toxaphene involves exposing chlorinated camphenes to UV-radiation, the congeners in the final mixture are resistant to degradation from direct photolysis (EPA 1976a; Korte et al. 1979).</p> <p>Rapaport and Eisenreich (1986) cited an atmospheric residence time of 46-70 days for the mixture.</p> <p>They noted that the toxaphene found in peat cores taken from remote regions in the northern United States and Canada was deposited from the atmosphere in a relatively untransformed state.</p> <p>5.3.2.2 Water</p> <p>Toxaphene is resistant to chemical and biological transformation in aerobic surface waters. It is not expected to undergo direct photolysis or photooxidation (EPA 1979a). Hydrolysis is also not an important fate process; a hydrolytic half-life of greater than 10 years for pH 5 to 8 and 25°C has been estimated (EPA 1976d).</p>

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Endrin	II	<b>0.001</b> (0.00007 - 0.02)	<p>Laboratory studies have indicated that one common mechanism for the transformation and degradation of endrin in air, water, and soil under field conditions is via <b>photochemical reactions and rearrangements resulting from ultraviolet irradiation from sunlight</b> (EPA 1985e; Zabik et al. 1971).</p> <p>Photochemical isomerization of endrin, primarily to the pentacyclic ketone commonly called delta ketoendrin or endrin ketone, was observed after exposure of thin layers of solid endrin on glass to sunlight (Burton and Pollard 1974). Minor amounts of endrin aldehyde were also formed in this reaction. <i>Results of seasonal studies indicated that this isomerization would proceed with a half-life of 5-9 days in intense summer sunlight, with complete conversion to the pentacyclic ketone in 15-19 days.</i></p> <p>Knoevenagel and Himmelreich (1976) reported that photodegradation of solid endrin in the laboratory proceeded with a half-life of 20-40 hours.</p> <p>In laboratory studies conducted by Zabik et al. (1971) on endrin formulations in hexane and cyclohexane (similar to those commonly used for pesticide applications), endrin was found to undergo photolytic dechlorination when exposed to ultraviolet radiation, yielding a pentachlorinated half-cage ketone as the major product. This degradation product was also detected in environmental samples.</p> <p>Endrin is also sensitive to transformation by heat, yielding primarily the pentacyclic ketone and endrin aldehyde at temperatures greater than 230°C (EPA 1979g; Phillips et al. 1962).</p> <p>5.3.2.1 Air</p> <p><b>Studies regarding photodegradation of endrin in the atmosphere have not been located.</b> Based on laboratory experiments on solid endrin (Burton and Pollard 1974) and on endrin in organic solvents (Zabik et al. 1971), it is likely that endrin in air will undergo photoisomerization to a ketoendrin, with minor amounts of endrin aldehyde also being formed. Endrin may also be transformed by heat in the atmosphere to the pentacyclic ketone and endrin aldehyde (Phillips et al. 1962).</p> <p>Laboratory studies of the fate of endrin in water samples suggest a significant degree of stability...</p> <p>Studies in which sealed water samples from the Little Miami River were exposed to sunlight and artificial fluorescent light showed no measurable degradation of endrin over an 8-week period (Eichelberger and Lichtenberg 1971).</p>

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Heptachlor / Heptachlor Epoxide	II	0.0003 Hept. (0.00002 - 0.004)	<p><b>Heptachlor may undergo direct photolysis in sunlight and is also susceptible to photosensitized reactions (Graham et al. 1973; Ivie et al. 1972).</b></p> <p>Heptachlor is hydrolyzed in surface water and distilled water to 1-hydroxychlordene. When heptachlor was added to a sample of river water maintained at room temperature and exposed to sunlight, only 25% remained after 1 week, and no heptachlor remained after the 2nd week. The 75% loss of heptachlor after 1 week corresponds to a half-life of 3.5 days. The products formed were identified as 1-hydroxychlordene and heptachlor epoxide. It was observed that an equilibrium exists at the end of 4 weeks between 1-hydroxychlordene and heptachlor epoxide, so that approximately 60% of the converted heptachlor remained as 1-hydroxychlordene and 40% was converted to the epoxide.</p> <p>When a 14C-heptachlor-treated model aquatic ecosystem was examined for transformation of heptachlor in water, the relative amounts of various transformation products in water were determined as the percentage of the total 14C label in the water sample. Heptachlor was found to decrease from 100% to approximately 10% of total 14C material in 1 day (Lu et al. 1975). After 1 day, 1-hydroxychlordene epoxide was present as 50% of the total 14C, rose to 70% on day 3, and then remained constant until day 13 of the experiment. The heptachlor hydrolysis product, 1-hydroxychlordene, reached a maximum of 10% of the total 14C at day 1 and decreased thereafter. <b>A relatively small proportion of heptachlor epoxide was formed.</b> Heptachlor epoxide was never found to be greater than 10% of the total 14C in the water sample. <b>The authors concluded that the major pathway of heptachlor in aquatic systems is rapid abiotic hydrolysis of heptachlor to 1-hydroxychlordene followed by metabolism to 1-hydroxychlordene epoxide (Lu et al. 1975).</b></p> <p>Loamy soils treated with heptachlor at 25 pounds per 5-inch acre, over a 5-year period from 1958 through 1962, contained about 5% of the applied dosages in the fall of 1968, primarily in the form of heptachlor epoxide. In addition to g-chlordane and nonachlor, which were present in the original heptachlor formulation, two toxic metabolites (heptachlor epoxide and a-chlordane) and three unidentified compounds were detected, thus indicating the breakdown in soils of heptachlor and related compounds (Lichenstein et al. 1970).</p>

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		<b>0.002</b> Hept. Epox. (0.0001 - 0.02)	<p>Heptachlor epoxide is converted to intermediate and final photoproducts when exposed to sunlight or ultraviolet light on the surface of plants (Podowski et al. 1979).</p> <p>From 40% to 50% conversion occurred in 4 hours on bean leaves treated with rotenone, an insecticide, acting as a photosensitizer.</p> <p>No detectable photoproducts (photoheptachlor epoxide) were formed in the absence of rotenone. The photolysis products were ketones.</p> <p>The intermediate photoproduct has a reduced toxicity in mice as compared to heptachlor epoxide, and it is completely nontoxic to houseflies. The final photoproduct is more toxic to flies and mice than the parent heptachlor epoxide (Ivie et al. 1972).</p> <p><b>The photoisomers of heptachlor epoxide are not expected to form in appreciable amounts in the environment unless a potent photosensitizer is present (Ivie et al. 1972).</b></p> <p>The photolysis of heptachlor epoxide as a solid (pressed) disk, as a powder, and as 0.5% heptachlor epoxide in a potassium bromide (a photosensitizer) disk was studied.</p> <p>The physical nature of the sample and the intensity of illumination affected the rate of photolysis. After 121 hours of exposure to sunlight in July, 93%, 98%, and 0% heptachlor epoxide remained in the solid disk, powder, and potassium bromide disk, respectively. <i>When a powdered sample of heptachlor epoxide was irradiated on a rooftop of an unspecified location from January through mid-September, degradation was almost negligible until May, then increased through July, reaching a maximum decomposition rate of 1% per day at the end of July. By the end of the experiment (8.5 months), 39% of the original sample has decomposed (Graham et al. 1973).</i></p> <p>When heptachlor epoxide was added to a sample of river water (pH 7.3-8) and to distilled water, it remained unchanged for 8 weeks. A half-life of at least 4 years was calculated for heptachlor epoxide (Eichelberger and Lichtenberg 1971).</p>

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Hexachloro-cyclohexane	II	<b>0.0006</b> ( $\alpha$ ) (0.00004 - 0.006)	<p>As mentioned earlier, g-HCH can be present in the air as vapor or sorbed to particulate matter. The widespread global distribution of HCH isomers is indicative of the persistence of g-HCH in the air. It appears that photodegradation or other degradation processes are not significant processes in the removal of g-HCH from air, as compared to rain-out or dry deposition.</p> <p><b>The structure of g-HCH and other isomers of HCH are such that the compounds would have very little absorption above the solar spectral region cutoff at 290 nm.</b></p>
		<b>0.002</b> ( $\beta$ ) (0.0001 - 0.01)	<p>However, Hamada et al. (1981) found that g-HCH underwent photodegradation to form two isomers of tetrachlorohexene and pentachlorohexane in propanol solution when irradiated with ultraviolet light produced by a low-pressure mercury lamp. Similar transformation of g-HCH and other isomers is thought to occur to some extent in the atmosphere.</p>
		<b>0.001</b> ( $\delta$ ) (0.00007 - 0.01)	<p>Water:</p> <p><b>Biodegradation is believed to be the dominant degradative process for g-HCH in aquatic systems, although hydrolysis and photolysis do occur.</b></p> <ul style="list-style-type: none"> <li>● Somewhat conflicting information is available on the rate of photolysis of g-HCH in water.               <ul style="list-style-type: none"> <li>● In the study by Saleh et al. (1982) discussed above, the authors also reported g-HCH first-order photolysis half-lives of 169, 1,791, and 1,540 hours at pH 9.3, 7.3, and 7.8, respectively. The adjusted mid-winter half-life of g-HCH in pure water was reported to be 1,560 hours.</li> <li>● However, in another study, g-HCH rapidly disappeared from a sterile aqueous solution when exposed to ultraviolet radiation in atmospheric nitrogen; less than 1% of the original amount was left in solution after 30 hours of exposure (Malaiyandi et al. 1982).</li> </ul> </li> <li>● Hydrolysis is not considered an important degradation process for g-HCH in aquatic environments under neutral pH conditions. However, under alkaline conditions, g-HCH is hydrolyzed fairly rapidly. Saleh et al. (1982) tested rates of hydrolysis of g-HCH in sterilized natural waters at 25°C and found that hydrolysis of g-HCH followed first-order kinetics with half-lives of 92 hours at pH 9.3, 648 hours at pH 7.8, and 771 hours at pH 7.3.</li> </ul>
		<b>0.003</b> ( $\gamma$ ) (0.0002 - 0.03)	

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Methoxychlor	II	0.1 (0.005 - 0.6)	<p>Data regarding the transformation and degradation of methoxychlor in air were not located.</p> <p>It has been estimated that the half-life for photooxidation in air may range from 1 to 11 hours (Howard 1991).</p> <p>5.3.2.2 Water</p> <p>Methoxychlor can be degraded in water by chemical, photochemical, and biological processes. Methoxychlor undergoes a spontaneous elimination reaction in aqueous solution to yield dehydrochlorinated products including methoxy-DDE (a proestrogenic derivative of methoxychlor discussed in Section 2.3.5). The half-life for the degradation of methoxychlor by this process was estimated to be approximately 1 year (Wolfe et al. 1977).</p> <p>Methoxychlor may also be oxidized by hydroxyl radicals or ozone in ozonated waters (Haag and Yao 1992; Yao and Haag 1991). The half-life of methoxychlor reaction with ozone <u>under ozonation conditions</u> was estimated to be 2.1 minutes.</p> <p><i>Methoxychlor is photochemically degraded by sunlight through loss of one chlorine atom to form a radical intermediate, which rearranges to the more stable methoxy-DDE (Zeppl et al. 1976).</i></p> <p>A dramatic difference in half-life was observed for the photochemical degradation of methoxychlor in distilled water (4.5 months) and natural water (2-5 hours).</p> <p>Methoxychlor was found to form adducts extensively with plant materials via a photochemically-induced radical mechanism (Schwack 1988).</p> <p>This observation may explain the dramatic differences in the half-life of methoxychlor in distilled and natural waters.</p>

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Pentachloro-phenol	II	0.0006 (0.00004 - 0.006)	<p>5.3.2.1 Air</p> <p>Atmospheric pentachlorophenol is transformed via photolysis; the compound is not expected to undergo free radical oxidation.</p> <hr/> <p><b>Atmospheric pentachlorophenol is probably photolyzed in the absence of water, although mechanisms for this reaction are not well known (Crosby and Hamadad 1971; Gab et al. 1975).</b></p> <p>Photolysis of sorbed or film-state pentachlorophenol in the presence of oxygen has also been observed (Gab et al. 1975). The reaction products were similar to those found in aqueous photolysis.</p> <p>No information was found regarding susceptibility of pentachlorophenol to free radical oxidation in the atmosphere. However, related compounds such as benzene, chlorobenzenes, and phenol have low reactivity with atmospheric hydroxy radicals; therefore, atmospheric oxidation of penta-chlorophenol is not expected.</p> <p>5.3.2.2 Water</p> <p><b>Photolysis and biodegradation are believed to be the dominant transformation processes for pentachlorophenol in aquatic systems.</b> Hydrolysis and oxidation are not important mechanisms for removal of the compound from surface waters.</p> <p>The molecular structure of pentachlorophenol is indicative of its stability to hydrolysis or oxidation (Callahan et al. 1979). Wong and Crosby (1981) reported no changes in pentachloro-phenol concentration in dark controls during their study of pentachlorophenol photodecomposition in water. Pentachlorophenol apparently did not hydrolyze in aqueous solutions at pH 3.3 or 7.3 when held at 26°C for up to 100 hours.</p> <p><b>Wong and Crosby (1981) reported that pentachlorophenol in aqueous solutions was photolyzed under laboratory ultraviolet (UV)-light irradiation with estimated half-lives of about 100 hours at pH 3.3 and 3.5 hours at pH 7.3.</b></p> <p>Photolysis of pentachlorophenol in aqueous solution following exposure to sunlight was also rapid; in laboratory experiments, concentrations of pentachloro-phenol in water were reduced from 9.3 ppm to 0.4 ppm in 24 hours and approached zero at the end of 48 hours (Arsenault 1976).</p> <p>In outdoor tests conducted with river water in man-made channels, Pignatello et al. (1983) demonstrated that photolysis of pentachlorophenol was rapid at the water surface (half-life of 0.70 hour at a depth of 0.5 cm). However, photolysis was greatly attenuated with increasing depth of the water column (half-life of 228 hours at a depth of 30 cm). Photolytic degradation accounted for a 5-28% decrease in the initial test concentration of the compound after 3 weeks.</p>

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<b>INDUSTRIAL / MISCELLANEOUS</b>			
Octachloro-styrene	I	0.003 (0.0001 - 0.04)	
3,3'-Dichloro-benzidene	II	0.9 (0.3 - 0.99)	<p>5.3.2.1 Air</p> <p>3,3'-DCB in the atmosphere may be photooxidized with hydroxyl radicals and ozone, but there were no quantitative data on reaction rates.</p> <p>Radding et al. (1977) estimated the persistence of "all benzidines" in the atmosphere by assuming a hydroxyl radical concentration of <math>8 \times 10^{-15}</math> mole/liter (an average value in a 24-hour day-night cycle). Treating the photooxidation process as a first-order reaction, the rate constant was <math>7.2 \times 10^{12}</math>/mole-hr and the corresponding half-life was 12 hours. This approach was based on data on the rates of reaction of hydroxyl radicals with olefins, aromatics, and alkanes in the atmosphere.</p> <p>The estimated half-life of 3,3'-DCB in air has ranged from 1 to 60 days (Shriner et al. 1978; EPA 1980b). Based on the reaction rate constant of photodegradation in the atmosphere, the half-life may be as little as two hours (DCMA 1989). There was no other information on the fate of atmospheric 3,3'-DCB.</p> <p>5.3.2.2 Water</p> <p>The limited information that is available suggest that 3,3'-DCB may photolyze yielding benzidine which is more photostable. It does not appear that the chemical is susceptible to other transformations in water.</p> <p>In a study reported by Sikka et al. (1978) and Banerjee et al. (1978), 3,3'-DCB was found to be extremely photolabile in water. 3,3'-DCB photolyzed yielding monochlorobenzidine, benzidine, and a number of colored, water-insoluble products. In natural sunlight, the half-life of 3,3'-DCB in water was approximately 90 seconds. While 3,3'-DCB is very rapidly photolyzed under environmental conditions, the process may yield benzidine, a relatively photostable carcinogen (Banerjee et al. 1978).</p> <p>There are no data to suggest that the hydrolysis of 3,3'-DCB is significant (Callahan et al. 1979). Mabey et al. (1982) proposed a hydrolysis-rate constant of 0/mole-hour for 3,3'-DCB.</p> <p>It has been speculated that aromatic amines can be oxidized in solution by organic radicals, but there are no actual data on reaction rates. Based on structural analogs, Radding et al. (1977) estimated that the half-life of such compounds in water is approximately 100 days, assuming a peroxy concentration of 10-10 mole/L in sunlit, oxygenated water. Based on the oxidation rates with similar compounds, Mabey et al. (1982) treated the direct oxidation of 3,3'-DCB by oxygen in solution as a first-order reaction, and estimated a reaction rate constant of less than <math>4 \times 10^7</math>/mole-hour. The oxidation rate constant with peroxy radicals was estimated to be approximately <math>4 \times 10^7</math>/mole-hour. However, no information was located that demonstrates that 3,3'-DCB is significantly oxidized in water.</p>

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<b>4,4'-Methylene bis (2-Chloro-aniline) "MBOCA"</b>	II	<b>0.009</b> (0.0005 - 0.1)	<p>5.3.2.1 Air</p> <p>The photooxidation half-life of MBOCA in air is estimated to be between 0.290 and 2.90 hours based on reactions with hydroxyl radicals (Howard et al. 1991), suggesting that this may be a significant fate process.</p> <p>5.3.2.2 Water</p> <p>The estimated photooxidation half-life of MBOCA in surface water is between 1.3 and 72 days; while in groundwaters, MBOCA may have a half-life of 8 weeks to 1 year (Howard et al. 1991). The estimated hydrolysis half-life of MBOCA in water at 25°C and pH 7 is more than 800 years (EPA 1988c).</p>
<b>4-Bromo-phenyl Phenyl Ether "4BPE"</b>	II	<b>0.0005</b> (0.00002 - 0.02)	
<b>Hexachloro-1,3-Butadiene "HCBD"</b>	II	<b>0.000005</b> (0.0000002 - 0.0001)	<p>5.3.2.1 Air</p> <p>No data were located regarding the transformation and degradation of hexachlorobutadiene in air.</p> <p>Based on the monitoring data, the tropospheric half-life of hexachlorobutadiene was estimated by one author to be 1.6 years in the northern hemisphere (Class and Ballschmiter 1987).</p> <p>However, analogy to structurally similar compounds such as tetrachloroethylene indicates that the half-life of hexachlorobutadiene may be as short as 60 days, predominantly due to reactions with photochemically produced hydroxyl radicals and ozone (Atkinson 1987; Atkinson and Carter 1984).</p> <p>Oxidation constants of &lt;103 and 6 (m • hr)-1 were estimated for reactions with singlet oxygen and peroxy radicals, respectively (Mabey et al. 1982).</p> <p>5.3.2.2 Water</p> <p>Data concerning the transformation and degradation of hexachlorobutadiene in waters are limited... Data regarding the hydrolysis or photolysis of hexachlorobutadiene in water were not located.</p>

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<b>CHLOROBENZENES</b>			
1,4-dichloro-benzene "pDCB"	II	0.000004 (0.0000003 - 0.000003)	<p>5.3.2.1 Air</p> <p>The main degradation pathway for 1,4-dichlorobenzene in air is reaction with photochemically generated hydroxyl radicals (Cuppitt 1980; EPA 1985).</p> <p>Reactions with ozone or other common atmospheric species are not expected to be significant (Atkinson et al. 1985; Cuppitt 1980).</p> <p>Therefore, the atmospheric lifetime of 1,4-dichlorobenzene may be predicted from an assumed hydroxyl radical concentration in air and the rate of reaction.</p> <p>The reported rate for reaction of hydroxyl radicals with 1,4-dichlorobenzene is <math>3 \times 10^{-3}</math> cm<sup>3</sup>/mol-sec (Atkinson et al. 1985; Singh et al. 1981), and the estimated atmospheric residence time for 1,4-dichlorobenzene is about 39 days (Singh et al. 1981).</p> <p>Since this degradation process is relatively slow, 1,4-dichlorobenzene may become widely dispersed, but is not likely to accumulate in the atmosphere.</p> <p>5.3.2.2 Water</p> <p>Biodegradation may be an important transformation process for 1,4-dichlorobenzene in water under aerobic, but not anaerobic, conditions (Bouwer and McCarty 1982, 1983, 1984; Spain and Nishino 1987; Tabak et al. 1981).</p> <p>Although volatilization of 1,4-dichlorobenzene may interfere with biodegradation studies, <sup>14</sup>C studies indicate that significant biodegradation of 1,4-dichlorobenzene does occur (Spain and Nishino 1987).</p> <p>5.3.2.3 Soil</p> <p><b>Based on its tendency to sublime, volatilization is the most likely fate process for 1,4-dichlorobenzene from surface soil.</b> Biodegradation by soil organisms and leaching to groundwater from subsurface soils may also occur (EPA 1985). However, no quantitative data on rate or extent of volatilization were located.</p>
Tetrachloro-benzenes 1234 TCB 1245 TCB 1235 TCB	II	0.000009 (1234TCB) (0.000006 - 0.0001)	
		0.000008 (1245TCB) (0.0000005 - 0.00006)	
		0.000004 (1235TCB) (0.0000003 - 0.00004)	
Pentachloro-benzene "PeCB"	II	0.00009 (0.000006 - 0.001)	

**Table D.4.-(1). Some Information about Atmospheric Photolysis  
(i.e., Destruction by UV Light) for Compounds Considered in this Study**

Chemical or Group	LVL	Estimated Fraction Adsorbed to Particles in Atm. (App. C) (1)	<b>Information Regarding Atmospheric Photolysis</b> All Information Imported Directly from ATSDR Toxicological Profiles (CD ROM version) unless otherwise indicated; References cited are as cited in the original (e.g. ATSDR) document. Time constraints did not allow the inclusion of these references in the bibliography for this report.
<b>Hexachlorobenzene "HCB"</b>	I	<b>0.0003</b> (0.00002 - 0.003)	<p>Few studies regarding atmospheric degradation of hexachlorobenzene have been located, probably because the atmosphere is not a significant reservoir of hexachlorobenzene.</p> <p>Photodegradation of hexachlorobenzene in its vapor phase, or as an adsorbable on silica gel, has been reported as <b>not</b> occurring when hexachlorobenzene was irradiated with ultraviolet radiation of wavelength 290 nm for 6 days; however, production of HC1 and CO<sub>2</sub> was observed when hexachlorobenzene was irradiated at 230 nm (Parlar 1978).</p> <p><b>In the troposphere, hexachlorobenzene is probably photochemically stable</b>, but degradation in the stratosphere by photodissociation by shorter-wavelength, higher-ultraviolet light may be a mechanism for atmospheric degradation.</p> <p>While not highly volatile, hexachlorobenzene can volatilize and is often studied in conjunction with the semi-volatile organochloro compounds (Ballschmiter and Wittlinger 1991; Lane et al. 1992). It is resistant to the types of hydrolysis reactions that can help degrade other organochlorines or organophosphates; and <b>with a half-life of about 90 days, it is not markedly subject to photolytic decay (EPA 1992b)</b>.</p>

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<b>POLYCHLORINATED DIBENZO-P-DIOXINS AND DIBENZOFURANS (PCDD/F'S)</b>			
2,3,7,8-TCDD	I	<b>0.6</b> (0.08 - 0.9)	5.3.2.1 Air  <b>No data regarding vapor phase photolysis of CDFs were located. In the absence of data, the half-lives of these compounds in the vapor phase have been estimated from aqueous phase photolysis data and it was concluded that photolysis is relatively unimportant, even when compared to reaction with hydroxyl radicals (with the possible exception of 1,3,6,8-tetraCDF) (Atkinson 1991).</b>  The loss of vapor phase CDFs by reactions with HO <sub>2</sub> radicals, NO <sub>3</sub> radicals and ozone has been estimated to be of negligible importance in the troposphere (Atkinson 1991).
2,3,7,8-TCDF	I	<b>0.3</b> (0.02 - 0.9)	
PeCDD/F's (penta-chloro-)	I	<b>0.9</b> (0.2 - 0.99)	
HxCDD/F's (hexa-chloro-)	I	<b>0.97</b> (0.6 - 1)	The estimated rate constants for the reactions of vapor phase CDFs with OH radicals are as follows (10-12 cm <sup>3</sup> /molecule-sec): tetraCDFs, 1.4-8.3; pentaCDFs, 1.0-4.3; hexaCDFs, 0.74-2.6; heptaCDFs, 0.53-0.92; and octaCDFs, 0.39. Using a 12-hour average daytime hydroxyl radical concentration of 1.5x10 <sup>6</sup> /cm <sup>3</sup> , the estimated tropospheric lifetimes of tetra-, penta-, hexa-, hepta-, and octaCDF are 1.9-11, 3.6-15, 5.9-22, 17-31, and 39 days, respectively.
HxCDD/F's (hepta-chloro-)	I	<b>0.99</b> (0.9 - 1)	The vapor phase reaction of CDFs with hydroxyl radicals is the dominant loss process and this loss process is more important for the lower, than the higher, chlorinated congeners, because the lifetimes due to this reaction are shorter for lower chlorinated congeners and the vapor phase concentrations of lower chlorinated congeners are higher.
OCDD/F's (octa-chloro-)	I	<b>1</b> (0.98 - 1)	Based on the available information, the reactions of hydroxyl radicals with particulate phase CDFs are insignificant and the principal air removal mechanism for CDFs is wet and dry deposition.
PCDD/F's (as a group)	I		Photodegradation of CDFs bound to atmospheric particles is not an important process in removing these compounds from air (Koester and Hites 1992).

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Chemical or Group	LVL	Estimated Fraction Adsorbed to Particles in Atm. (App. C) (1)	Information Regarding Atmospheric Photolysis All Information Imported Directly from ATSDR Toxicological Profiles (CD ROM version) unless otherwise indicated; References cited are as cited in the original (e.g. ATSDR) document. Time constraints did not allow the inclusion of these references in the bibliography for this report.
<b>POLYCHLORINATED BIPHENYLS (PCB'S)</b>			
Cl <sub>1</sub> -PCB		<b>0.00007 - 0.00014</b> (0.000001 - 0.01)	The ability of PCBs to be degraded or transformed in the environment depends on the degree of chlorination of the biphenyl molecule as well as on the isomeric substitution pattern (Callahan et al. 1979; EPA 1988a; Leifer et al. 1983). In general, the persistence of PCB congeners increases as the degree of chlorination increases.  5.3.2.1 Air
Cl <sub>2</sub> -PCB		<b>0.0004 - 0.0020</b> (0.000007 - 0.2)	In the atmosphere, the vapor-phase reaction of PCBs with hydroxyl radicals (which are photochemically formed by sunlight) may be the dominant transformation process.
Cl <sub>3</sub> -PCB		<b>0.001 - 0.012</b> (0.00002 - 0.6)	The estimated tropospheric half-lives for this reaction with various PCB isomers are: monochlorobiphenyl, 3.5-7.6 days; dichlorobiphenyl, 5.5-11.8 days; trichlorobiphenyl, 9.7-20.8 days; tetrachlorobiphenyl, 17.3-41.6 days; and pentachlorobiphenyl, 41.6-83.2 days (Atkinson 1987).
Cl <sub>4</sub> -PCB		<b>0.003 - 0.069</b> (0.00006 - 0.94)	Photochemical studies conducted with a number of chlorobiphenyl congeners and commercial PCB mixtures in aqueous suspension, thin film, or vapor state under simulated and natural sunlight conditions resulted in several degradative reactions that produced dechlorination, polymerization, and polar (hydroxy- and carboxy-) products (Hutzinger et al. 1972). Therefore, photolytic degradation of PCBs in the atmosphere is possible. However, the rates of these reactions with natural sunlight were not reported.
Cl <sub>5</sub> -PCB		<b>0.03 - 0.27</b> (0.0003 - 0.99)	5.3.2.2 Water
Cl <sub>6</sub> -PCB		<b>0.04 - 0.74</b> (0.0005 - 0.999)	<i>In water, transformation processes such as hydrolysis and oxidation do not significantly degrade PCBs (Callahan et al. 1979). Photolysis appears to be the only viable chemical degradation process in water. PCBs containing up to six chlorine substitutions do not significantly absorb sunlight, and the estimated photolysis half-lives of mono- through tetrachlorobiphenyls with summer sunlight at shallow water depth (&lt;0.5 m) range from 17 to 210 days. Photolysis rates with sunlight are even slower during winter. Nonetheless, as the number of chlorine substitutions increases, the light absorption band shifts towards longer wavelengths, and the photolysis rate for hepta- through decachlorinated biphenyls increases. The estimated photolysis half-life of Aroclor 1268 with summer sunlight is 0.1 days, compared to 23 days for Aroclor 1232 (Leifer et al. 1983). However, these results must be used with caution since the solvent used was predominantly acetonitrile (75%) and, therefore, the experiment does not correspond with environmental conditions. More reliable photolysis data are needed to estimate rates of photolysis in aqueous media in the presence of sunlight.</i>
Cl <sub>7</sub> -PCB		<b>0.25 - 0.91</b> (0.003 - 1.000)	The photolysis rates for PCBs can be enhanced by a factor of 311, in the presence of sodium borohydride (Epling et al. 1988). Therefore, photolysis in the presence of sodium borohydride may be useful as a method for destruction of PCBs in water. The exposure of 0.08 mg/L aqueous solution of Aroclor 1248 to sunlight in the presence of a titanium dioxide suspension (50 g/L) decreased the total PCB concentration to 23% of original in 2 hours and to 13% of original in 4 hours (Zhang et al. 1993). Although the intermediate and final products of photocatalysis were not identified, it was suggested by the authors of other related studies that photolysis resulted in complete mineralization of PCB.
Cl <sub>8</sub> -PCB		<b>0.85 - 0.95</b> (0.05 - 1.00)	
Cl <sub>9</sub> -PCB		<b>0.93</b> (0.09 - 1.00)	
PCB's as a group	I		

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<b>POLYCYCLIC AROMATIC HYDROCARBONS</b>			
Naphthalene "Naph"		<b>0.000002</b> (0.000001 - 0.00002)	
Ace-naphthalene "Acn"		<b>0.00005</b> (0.000003 - 0.0006)	
Ace-naphthylene "Acl"		<b>0.00002</b> (0.000001 - 0.0002)	
Fluorene "Flr"		<b>0.0001</b> (0.000007 - 0.001)	
Phenanthrene "Phen"	II	<b>0.0008</b> (0.00004 - 0.01)	
Anthracene "Anth"	II	<b>0.001</b> (0.00006 - 0.01)	
Pyrene "Pyr"		<b>0.007</b> (0.0004 - 0.08)	
Fluoranthene "Fln"		<b>0.01</b> (0.0005 - 0.1)	
Chrysene "Chr"		<b>0.4</b> (0.04 - 0.9)	
Benz (a) Anthracene "BaA"	II	<b>0.5</b> (0.05 - 0.95)	
Benzo (b) Fluoranthene "BbF"		<b>0.05</b> (0.002 - 0.5)	
Benzo (j) Fluoranthene "BjF"		<b>0.7</b> (0.08 - 0.97)	
Benzo (k) Fluoranthene "BkF"		<b>0.96</b> (0.5 - 1)	
Benzo (a) Pyrene "BaP"	I	<b>0.8</b> (0.2 - 0.99)	<p>[HSDB]: When released to air it may be subject to direct photolysis, although adsorption to particulates apparently can retard this process. It may also be removed by reaction with O<sub>3</sub> (half-life 37 min) and NO<sub>2</sub> (half-life 7 days), and an estimated half-life for reaction with photochemically produced hydroxyl radicals is 21.49 hr.(SRC) [CITATION] **PEER REVIEWED**</p> <p>[HSDB]: Half-life for reaction of a thin film of BaP with 0.19 ppm O<sub>3</sub> is 37 min and for reaction of adsorbed BaP with NO<sub>2</sub> is 7 days. The estimated half-life for reaction with photochemically produced hydroxyl radicals is 21.49 hr.</p>

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<b>Benzo (e) Pyrene "BeP"</b>		<b>0.8</b> (0.1 - 0.99)	
<b>Perylene "Per"</b>	II	<b>0.95</b> (0.5 - 1)	
<b>Benzo (g,h,i) Perylene "BgP"</b>	II	<b>0.96</b> (0.5 - 1)	
<b>Dibenz (a,h) Anthracene "dBA"</b>		<b>1</b> (0.98 - 1)	
<b>Indeno (1,2,3-c,d) Pyrene "IPyr"</b>		<b>0.99</b> (0.9 - 1)	
<b>Dinitro-pyrenes "DNPs"</b>	II	<b>0.4</b> (0.03 - 0.9)	<p>The processes that transform and degrade PAHs in the atmosphere include photolysis and reaction with NOx, N2O5, OH, ozone, sulfur dioxide, and peroxyacetyl nitrate (Baek et al. 1991; NRC 1983). Possible atmospheric reaction products are oxy-, hydroxy-, nitro- and hydroxynitro-PAH derivatives (Baek et al. 1991). <b>Photochemical oxidation of a number of PAHs has been reported with the formation of nitrated PAHs</b>, quinones, phenols, and dihydrodiols (Holloway et al. 1987; Kamens et al. 1986). <b>Some of these breakdown products are mutagenic</b> (Gibson et al. 1978). Reaction with ozone or peroxyacetyl nitrate yields diones; <b>nitrogen oxide reactions yield nitro and dinitro PAHs</b>. Sulfonic acids have also been formed from reaction with sulfur dioxide.</p> <p>The reactions of PAHs, including fluoranthene and pyrene, with the OH radical (in the presence of NOx) and with N2O5 led to the formation of nitroarenes that have been identified in the ambient air. As a class of compounds, the nitrated PAHs have been found to be much more mutagenic than their parent PAHs (Kamens et al. 1993).</p>

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PAH's (as a group)	II		<p>The processes that transform and degrade PAHs in the atmosphere include photolysis and reaction with NOx, N2O5, OH, ozone, sulfur dioxide, and peroxyacetyl nitrate (Baek et al. 1991; NRC 1983).</p> <p>Most PAHs in the atmosphere are associated with particulates (Baek et al. 1991).</p> <p>Vu-Duc and Huynh (1991) describe two types of chemical reactions that appear to be the predominant mode of transformation of these PAHs:</p> <ul style="list-style-type: none"> <li>(1) reactions between PAHs adsorbed on the particle surfaces and oxidant gases like NO2, O3, and SO3 that do not appear to be influenced by exposure to UV irradiation and</li> <li>(2) photooxidation of PAHs irradiated either under solar radiation or simulated sunlight which produces a variety of oxidized derivatives such as quinones, ketones, or acids.</li> </ul> <p><b>Kamens et al. (1990) estimate that, even in highly polluted air, photolysis is the most important factor in the decay of particle-sorbed PAHs in the atmosphere, followed by reaction with NO2, N2O5, and HNO3.</b></p> <p>The rates of homogeneous vapor phase chemical reactions are usually faster than heterogeneous chemical reactions of particulate PAHs with sunlight and oxidants in the atmosphere, particularly due to light shielding and stabilizing (toward both oxidation and photolysis) effects in the adsorbed state (Behymer and Hites 1988).</p> <p>PAHs have a wide range of volatilities and therefore are distributed in the atmosphere between the gas and particle phases. The 2-4 ring PAHs exist, at least partially, in the gas phase.</p> <p>Atkinson et al. (1991) calculated atmospheric lifetimes (1.44 times the half-life) of several gas-phase PAHs due to reactions with measured or estimated ambient concentrations of OH radicals, NO3 radicals, N2O5, and O3. Their laboratory studies showed that, for PAHs not containing cyclopenta-fused rings, the major gas-phase process resulting in atmospheric loss will be reaction with the OH radical. Calculated atmospheric lifetimes for acenaphthene, acenaphthylene, phenanthrene, and anthracene were on the order of a few hours. Nighttime reaction with N2O5 was estimated to be a minor source of atmospheric loss.</p>
<b>References and Notes for above Table</b>			
(1) Vapor Particle Partition Estimates Included here for convenience: <ul style="list-style-type: none"> <li>• Central Estimate (<b>bold</b>) T = 290°K; Aerosol surface area = 3.5e-6 cm<sup>2</sup>/cm<sup>3</sup></li> <li>• RANGE (in parentheses): 310 to 260 °K; 4.2e-7 to 1.1e-5 cm<sup>2</sup>/cm<sup>3</sup></li> </ul>			

## **Appendix D.5.**

### **Results of a Literature Search for Measurements of Rate Constants for the Reaction of Hydroxyl Radical with Organic Compounds in the Atmosphere Made by Atkinson and Colleagues**

(sorted by year: 1983 - 1996)

Atkinson, R., S. M. Aschmann, et al. (1983). "Kinetics Of the Reactions Of O<sub>3</sub> and OH Radicals With Furan and Thiophene At 298 +/- 2 K." International Journal Of Chemical Kinetics **15**(1): 51-61.

Biermann, H. W., H. Macleod, et al. (1985). "Kinetics Of the Gas-Phase Reactions Of the Hydroxyl Radical With Naphthalene, Phenanthrene, and Anthracene." Environmental Science & Technology **19**(3): 244-248.

Atkinson, R. and S. M. Aschmann (1985). "Rate Constants For the Gas-Phase Reaction Of Hydroxyl Radicals With Biphenyl and the Monochlorobiphenyls At 295+/-1-K." Environmental Science & Technology **19**(5): 462-464.

Atkinson, R. (1985). "Kinetics and Mechanisms Of the Gas-Phase Reactions Of the Hydroxyl Radical With Organic-Compounds Under Atmospheric Conditions." Chemical Reviews **85**(1): 69-201.

Atkinson, R. and W. P. L. Carter (1986). "The Atmospheric Chemistry Of Aromatic-Hydrocarbons - the Status Of Experimental-Data." Abstracts Of Papers Of the American Chemical Society **192**(SEP): 1-ENVR.

Tuazon, E. C., H. Macleod, et al. (1986). "Alpha-Dicarbonyl Yields From the NO<sub>x</sub>-Air Photooxidations Of a Series Of Aromatic-Hydrocarbons In Air." Environmental Science & Technology **20**(4): 383-387.

Atkinson, R. (1986). "Estimations Of OH Radical Rate Constants From H-Atom Abstraction From C-H and O-H Bonds Over the Temperature-Range 250-1000-K." International Journal Of Chemical Kinetics **18**(5): 555-568.

Lurmann, F. W., A. C. Lloyd, et al. (1986). "A Chemical Mechanism For Use In Long-Range Transport Acid Deposition Computer Modeling." Journal Of Geophysical Research-Atmospheres **91**(D10): 905-936.

Arey, J., B. Zielinska, et al. (1986). "The Formation Of Nitro-PAH From the Gas-Phase Reactions Of Fluoranthene and Pyrene With the OH Radical In the Presence Of NO<sub>x</sub>." Atmospheric Environment **20**(12): 2339-2345.

Atkinson, R. (1987). "Estimation Of OH Radical Reaction-Rate Constants and Atmospheric Lifetimes For Polychlorobiphenyls, Dibenzo-Para-Dioxins, and Dibenzofurans." Environmental Science & Technology **21**(3): 305-307.

Atkinson, R., J. Arey, et al. (1987). "Kinetics and Products Of the Gas-Phase Reactions Of OH Radicals and N<sub>2</sub>O<sub>5</sub> With Naphthalene and Biphenyl." Environmental Science & Technology **21**(10): 1014-1022.

Atkinson, R. (1987). "Estimation Of Gas-Phase Hydroxyl Radical Rate Constants For Organic-Chemicals." Abstracts Of Papers Of the American Chemical Society **193**(APR): 53-ENVR.

Atkinson, R., S. M. Aschmann, et al. (1987). "Kinetics Of the Gas-Phase Reactions Of NO<sub>3</sub> Radicals With

a Series Of Alkynes, Haloalkenes, and Alpha,Beta-Unsaturated Aldehydes." International Journal Of Chemical Kinetics **19**(4): 299-307.

Atkinson, R. (1987). "A Structure-Activity Relationship For the Estimation Of Rate Constants For the Gas-Phase Reactions Of OH Radicals With Organic-Compounds." International Journal Of Chemical Kinetics **19**(9): 799-828.

Atkinson, R., S. M. Aschmann, et al. (1988). "Rate Constants For the Gas-Phase Reactions Of the NO<sub>3</sub> Radical With a Series Of Organic-Compounds At 296+/-2-K." Journal Of Physical Chemistry **92**(12): 3454-3457.

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Atkinson, R. and S. M. Aschmann (1989). "Rate Constants For the Gas-Phase Reactions Of the OH Radical With a Series Of Aromatic-Hydrocarbons At 296 +/- 2-K." International Journal Of Chemical Kinetics **21**(5): 355-365.

Arey, J., B. Zielinska, et al. (1989). "Nitroarene Products From the Gas-Phase Reactions Of Volatile Polycyclic Aromatic-Hydrocarbons With the OH Radical and N<sub>2</sub>O<sub>5</sub>." International Journal Of Chemical Kinetics **21**(9): 775-799.

Atkinson, R. (1990). "Gas-Phase Tropospheric Chemistry Of Organic-Compounds - a Review." Atmospheric Environment Part a-General Topics **24**(1): 1-41.

Arey, J., R. Atkinson, et al. (1990). "Product Study Of the Gas-Phase Reactions Of Monoterpenes With the OH Radical In the Presence Of NO<sub>x</sub>." Journal Of Geophysical Research-Atmospheres **95**(D11): 18539-18546.

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Atkinson, R. (1991). "Kinetics and Mechanisms Of the Gas-Phase Reactions Of the NO<sub>3</sub> Radical With Organic-Compounds." Journal Of Physical and Chemical Reference Data **20**(3): 459-507.

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